Case/Application number: 10598826
Priority Filing Date:
Format for Search Results: No selection
Meaning of unusual acronyms or initialisms:

Identify the novelty:

Additional comments:
Please search the following attached claims (claims 1, 2, 11 and 12).

```
=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 16:20:31 ON 15 AUG 2008
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FILE COVERS 1907 - 15 Aug 2008  VOL 149 ISS 8
FILE LAST UPDATED: 14 Aug 2008  (20080814/ED)

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reclassification data for the second quarter of 2008.

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 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

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=> d stat que l28
L23             STR
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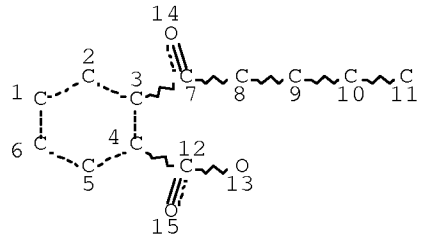

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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE
L25 128 SEA FILE=REGISTRY SSS FUL L23
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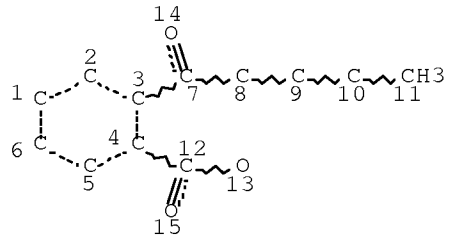

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
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GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE
L27 38 SEA FILE=REGISTRY SUB=L25 SSS FUL L26
L28 40 SEA FILE=HCAPLUS ABB=ON PLU=ON L27

=> d ibib abs hitstr l28 1-40

L28 ANSWER 1 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:1055762 HCAPLUS Full-text
DOCUMENT NUMBER: 147:468949
TITLE: Dipole-LUMO/Dipolarophile-HOMO Controlled Asymmetric Cycloadditions of Carbonyl Ylides Catalyzed by Chiral Lewis Acids
AUTHOR(S): Suga, Hiroyuki; Ishimoto, Daisuke; Higuchi, Satoshi; Ohtsuka, Motoo; Arikawa, Tadashi; Tsuchida, Teruko; Kakehi, Akikazu; Baba, Toshihide
CORPORATE SOURCE: Department of Chemistry and Material Engineering, Faculty of Engineering, Shinshu University, Wakasato, Nagano, 380-8553, Japan
SOURCE: Organic Letters (2007), 9(21), 4359-4362
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:468949
AB We have found the first successful example of reverse-electron-demand dipole-LUMO/dipolarophile-HOMO controlled cycloaddn. reactions between carbonyl

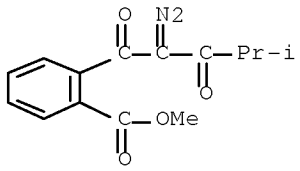
ylides, which were generated from o-methoxycarbonyl-α- diazoacetophenone and their acyl derivs. as precursors, and vinyl ether derivs. with high levels of asym. induction (97-77% ee) using chiral 2,6-(oxazolinyl)pyridine-Eu(III) or binaphthyldiimine-Ni(II) complexes as chiral Lewis acid catalysts.

IT 952687-64-8

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(dipole-LUMO/dipolarophile-HOMO controlled asym. cycloaddns. of carbonyl ylides catalyzed by chiral Lewis acids)

RN 952687-64-8 HCAPLUS

CN Benzoic acid, 2-(2-diazo-4-methyl-1,3-dioxopentyl)-, methyl ester (CA INDEX NAME)



REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 2 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:980459 HCAPLUS Full-text

DOCUMENT NUMBER: 149:9951

TITLE: Design, synthesis and activity evaluation of novel selective serotonin reuptake inhibitors

AUTHOR(S): Yang, Jing; Wang, Xiao-Fang; Du, Guan-Hua; Qin, Fang; Wen, Hui; Yang, Guang-Zhong

CORPORATE SOURCE: Institute of Materia Medica, Chinese Academy of Medical Sciences & Peking Union Medical College, Beijing, 100050, Peop. Rep. China

SOURCE: Gaodeng Xuexiao Huaxue Xuebao (2007), 28(8), 1503-1507
CODEN: KTHPDM; ISSN: 0251-0790

PUBLISHER: Gaodeng Jiaoyu Chubanshe

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

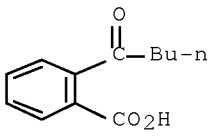
AB During the past two decades, selective serotonin reuptake inhibitors (SSRIs) have been proved to be a safer and more effective resistance than the first-generation antidepressants (TCAs and MAOIs), and have gained incredible popularity. Based on the conformation anal. and pharmacophore information of SSRIs, flexible database searching from the NCI-3D and Maybridge-3D database was performed. Three classes of the new compds. structures were designed and 27 analogs were prepared and evaluated as potential antidepressant agents. Biphenylbenzamidine derivative showed good activity of affinity to the 5-HT transporter. It can be used as the leader structure for drug design with the objective of making more potent inhibitors against 5-HT transporter.

IT 550-37-8P 64624-87-9P

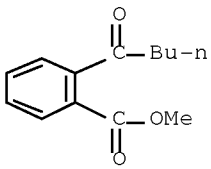
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(design, synthesis and evaluation of selective serotonin reuptake inhibitors)

RN 550-37-8 HCAPLUS

CN Benzoic acid, 2-(1-oxopentyl)- (CA INDEX NAME)



RN 64624-87-9 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)-, methyl ester (CA INDEX NAME)

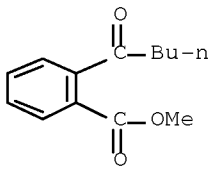


L28 ANSWER 3 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:833854 HCAPLUS Full-text
DOCUMENT NUMBER: 148:315535
TITLE: High-performance liquid chromatography with atmospheric pressure chemical ionization and electrospray ionization mass spectrometry for analysis of Angelica sinensis
AUTHOR(S): Wang, Ya-Li; Liang, Yi-Zeng; Chen, Ben-Mei
CORPORATE SOURCE: Research Center of Modernization of Chinese Herbal Medicines, Central South University, Changsha, 410083, Peop. Rep. China
SOURCE: Phytochemical Analysis (2007), 18(4), 265-274
CODEN: PHANEL; ISSN: 0958-0344
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB An HPLC-PAD-API/MS method for analyzing the chemical constituents of Angelica sinensis (A. sinensis) has been developed. ESI and APCI spectra, in both pos. ion and neg. ion modes, provided very useful information concerning the mol. wts. of detected compds. By comparing the retention times, UV spectra, mass spectra and mol. wts. of detected compds. with those published in literature, 15 constituents of A. sinensis could be tentatively identified. This technique involving combined MS information may provide an objective, reliable and rapid anal. method for the quality control and database research of traditional Chinese medicines.

IT 64624-87-9
RL: ANT (Analyte); NPO (Natural product occurrence); THU (Therapeutic use); ANST (Analytical study); BIOL (Biological study); OCCU (Occurrence); USES (Uses)
(Angelica sinensis anal. by high-performance liquid chromatog. with atmospheric pressure chemical ionization and electrospray ionization mass spectrometry)

RN 64624-87-9 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)-, methyl ester (CA INDEX NAME)



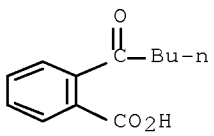
REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 4 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:809095 HCAPLUS Full-text
DOCUMENT NUMBER: 148:517475
TITLE: Stereoselective synthesis of 3-butylphthalide via CBS catalytic reduction
AUTHOR(S): Xu, Geng; Liu, Zhan Zhu; Yang, Jing Hua; Chen, Shi Zhi; Yang, Hui Ying
CORPORATE SOURCE: Institute of Materia Medica, Peking Union Medical College and Chinese Academy of Medical Science, Beijing, 100050, Peop. Rep. China
SOURCE: Chinese Chemical Letters (2007), 18(6), 653-655
CODEN: CCLEE7; ISSN: 1001-8417
PUBLISHER: Chinese Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

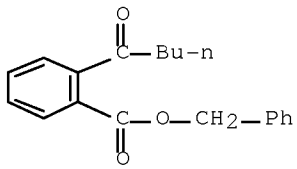
AB Optically active 3-butylphthalide of high enantiomeric excesses (≤93% ee) was synthesized by reduction of 2-pentanoylbenzoic ester with borane using B-methoxyoxazaborolidine as the chiral catalyst.

IT 550-37-8P, 2-Pentanoylbenzoic acid 1021950-15-1P, Benzyl 2-pentanoylbenzoate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(asym. synthesis of butylphthalide via reduction with oxazaborolidine catalyst)

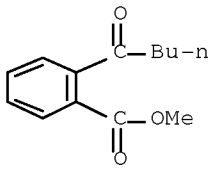
RN 550-37-8 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)- (CA INDEX NAME)



RN 1021950-15-1 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)-, phenylmethyl ester (CA INDEX NAME)



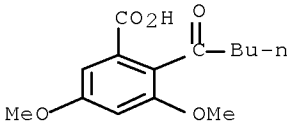
IT 64624-87-9P, Methyl 2-pentanoylbenzoate
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. synthesis of butylphthalide via reduction with oxazaborolidine catalyst)
RN 64624-87-9 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)-, methyl ester (CA INDEX NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 5 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:602595 HCAPLUS Full-text
DOCUMENT NUMBER: 147:180528
TITLE: Rational design of inhibitors of VirA-VirG two-component signal transduction
AUTHOR(S): Maresh, Justin; Zhang, Jin; Tzeng, Yih-Ling; Goodman, Nora A.; Lynn, David G.
CORPORATE SOURCE: Department of Chemistry, Center for Fundamental and Applied Molecular Evolution, Emory University, Atlanta, GA, 30322, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2007), 17(12), 3281-3286
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB VirA-VirG two-component system regulates the vir (virulence) operon in response to specific host factors (xenognosins) in the plant pathogen Agrobacterium tumefaciens. Using whole cell assays, stable inhibitors inspired by the labile natural benzoxazinone inhibitor HDMBOA are developed. It is found that aromatic aldehydes represent a minimal structural unit for activity. In particular, 3-hydroxy-4,6-dimethoxy-3H- isobenzofuran-1-one (HDI) was found to have the highest activity, making it the most potent developed inhibitor of virulence gene expression in Agrobacterium.
IT 944558-07-0
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study)
(rational design of inhibitors of VirA-VirG two-component signal

transduction based on maize root HDMBOA)
RN 944558-07-0 HCAPLUS
CN Benzoic acid, 3,5-dimethoxy-2-(1-oxopentyl)- (CA INDEX NAME)

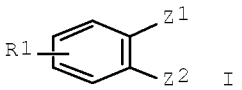


REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 6 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:1261607 HCAPLUS Full-text
DOCUMENT NUMBER: 144:6574
TITLE: Preparation of o-acylbenzoic acid derivatives from phthalic acid diesters
INVENTOR(S): Nishizawa, Yoshinori; Ichinose, Susumu
PATENT ASSIGNEE(S): Kao Corp., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

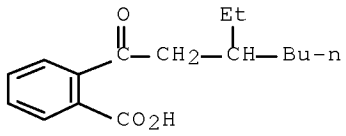
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2005330218	A	20051202	JP 2004-149474	20040519
PRIORITY APPLN. INFO.:			JP 2004-149474	20040519
OTHER SOURCE(S):	CASREACT 144:6574; MARPAT 144:6574			

GI



AB The derivs. I [R1 = H, halo, lower alkyl, lower alkoxy; Z1 = COR2 (R2 = alkyl); Z2 = CO2H], useful as intermediates for bioactive 3-substituted phthalides, are prepared by reacting R2MgX (R2 = same as above) with an excess amount of I [R1 = same as above; Z1, Z2 = CO2L (L = lower alkyl)] and hydrolyzing the resulting products. Thus, a THF/toluene solution of Me(CH2)7MgBr was added dropwise to a THF/toluene solution of 388.4 g o-C6H4(CO2Me)2 at 5° to give 134.6 g o-Me(CH2)7COC6H4CO2H.
IT 106462-12-8P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of o-acylbenzoic acids from phthalic acid diesters and Grignard reagents)
RN 106462-12-8 HCAPLUS

CN Benzoic acid, 2-(3-ethyl-1-oxoheptyl)- (CA INDEX NAME)

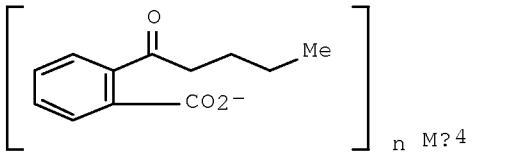


L28 ANSWER 7 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:1026918 HCAPLUS Full-text
DOCUMENT NUMBER: 143:299115
TITLE: Novel 2-(α-n-pentanonyl)benzoates, their preparation and use
INVENTOR(S): Liu, Quanzhi; Yang, Wenbin; Qin, Hua; Zhao, Xingkai; Ma, Xisheng
PATENT ASSIGNEE(S): Team Academy of Pharmaceutical Science, Peop. Rep. China
SOURCE: PCT Int. Appl., 35 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005087701	A1	20050922	WO 2004-CN602	20040604
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CN 1560018	A	20050105	CN 2004-10007520	20040312
EP 1734031	A1	20061220	EP 2004-738206	20040604
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LI, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
JP 2007528878	T	20071018	JP 2007-502170	20040604
US 20070203233	A1	20070830	US 2006-598826	20060912
KR 809778	B1	20080304	KR 2006-720046	20060927

PRIORITY APPLN. INFO.: CN 2004-10007520 A 20040312
WO 2004-CN602 W 20040604

GI



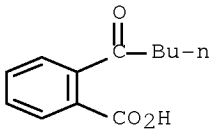
I

AB The present invention relates to novel compds. 2-(α-n- pentanonyl)benzoates I (where n = 1, 2; M = Na+, Ca+, K+, Li+, iso-Pr amine, N,N'-Dibenzyl ethylenediamine, Benzyl amine,(S)-α-Me benzyl amine), their preparation method, the pharmaceutical composition containing the same, and their use in preparing the medicine for preventing and/or treating cardioischemia/cerbroischemia, thrombus and disorder of cardiac/cerebral circulation.

IT 864856-61-1P
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(novel 2-(α -n-pentanonyl)benzoates, their preparation and use)

RN 864856-61-1 HCAPLUS

CN Benzoic acid, 2-(1-oxopentyl)-, sodium salt (1:1) (CA INDEX NAME)

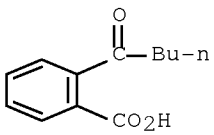


● Na

IT 864856-62-2P 864856-63-3P 864856-64-4P
864856-65-5P 864856-66-6P 864856-67-7P
864856-68-8P 864856-69-9P 864856-70-2P
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(novel 2-(α -n-pentanonyl)benzoates, their preparation and use)

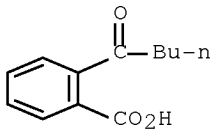
RN 864856-62-2 HCAPLUS

CN Benzoic acid, 2-(1-oxopentyl)-, potassium salt (1:1) (CA INDEX NAME)



● K

RN 864856-63-3 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)-, calcium salt (2:1) (CA INDEX NAME)

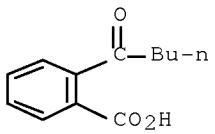


●1/2 Ca

RN 864856-64-4 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)-, compd. with N,N'-bis(phenylmethyl)-1,2-ethanediamine (2:1) (9CI) (CA INDEX NAME)

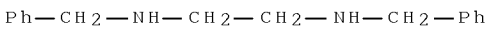
CM 1

CRN 550-37-8
CMF C12 H14 O3



CM 2

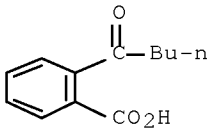
CRN 140-28-3
CMF C16 H20 N2



RN 864856-65-5 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)-, compd. with 2-methyl-2-propanamine (1:1) (CA INDEX NAME)

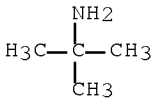
CM 1

CRN 550-37-8
CMF C12 H14 O3



CM 2

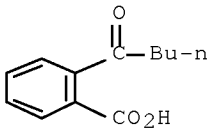
CRN 75-64-9
CMF C4 H11 N



RN 864856-66-6 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)-, compd. with benzenemethanamine (1:1) (CA INDEX NAME)

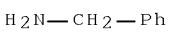
CM 1

CRN 550-37-8
CMF C12 H14 O3



CM 2

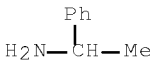
CRN 100-46-9
CMF C7 H9 N



RN 864856-67-7 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)-, compd. with α-methylbenzenemethanamine (1:1) (CA INDEX NAME)

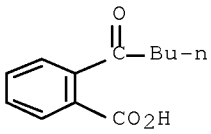
CM 1

CRN 618-36-0
CMF C8 H11 N

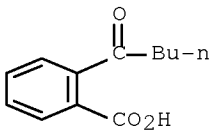


CM 2

CRN 550-37-8
CMF C12 H14 O3

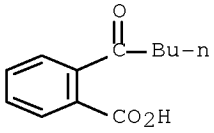


RN 864856-68-8 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)-, zinc salt (2:1) (CA INDEX NAME)



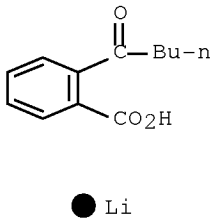
●1/2 Zn

RN 864856-69-9 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)-, magnesium salt (2:1) (CA INDEX NAME)

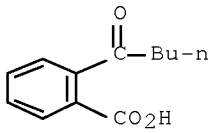


●1/2 Mg

RN 864856-70-2 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)-, lithium salt (1:1) (CA INDEX NAME)

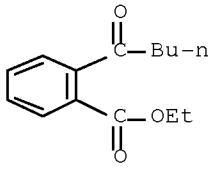


IT 550-37-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(novel 2-(α -n-pentanonyl)benzoates, their preparation and use)
RN 550-37-8 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)- (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 8 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:1000504 HCAPLUS Full-text
DOCUMENT NUMBER: 141:242819
TITLE: Product class 4: organometallic complexes of copper
AUTHOR(S): Heaney, H.; Christie, S.
CORPORATE SOURCE: Dept. of Chemistry, University of Loughborough, Loughborough, LE11 3TU, UK
SOURCE: Science of Synthesis (2004), 3, 305-662
CODEN: SSCYJ9
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review. The use of copper and related complexes in applications to organic synthesis is reviewed.
IT 131379-20-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(applications of copper and organocopper complexes to organic synthesis)
RN 131379-20-9 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)-, ethyl ester (CA INDEX NAME)

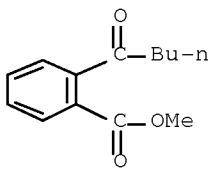


REFERENCE COUNT: 1706 THERE ARE 1706 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 9 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:129893 HCAPLUS Full-text
DOCUMENT NUMBER: 139:68703
TITLE: Ruthenium(II)-catalyzed asymmetric transfer hydrogenation of carbonyl compounds with 2-propanol and ephedrine-type ligands
AUTHOR(S): Everaere, Kathelyne; Mortreux, Andre; Carpentier, Jean-Francois
CORPORATE SOURCE: Laboratoire de Catalyse de Lille, UPRESA 8010 CNRS, Villeneuve d'Ascq, 59652, Fr.
SOURCE: Advanced Synthesis & Catalysis (2003), 345(1+2), 67-77
CODEN: ASCAF7; ISSN: 1615-4150
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:68703

AB The development and application of Noyori's type catalysts based on ruthenium-arene complexes and simple chiral β-amino alcs. derived from ephedrine for the asym. transfer hydrogenation of 2-propanol to carbonyl substrates are studied. The influence of key parameters of the catalyst system has been studied systematically, resulting in particular in the design of the novel ligand (4-biphenylmethyl)norephedrine. The catalytic precursors and true active species could be isolated for the first time, enabling a complete structural description of the catalytic cycle and of probable deactivation pathways. Highly effective applications of those catalysts systems, i.e., the asym. redns. of simple aryl ketones and aryl β-keto esters, the synthesis of chiral phthalides and syn-β,δ-dihydroxy esters, are described.

IT 64624-87-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. transfer hydrogenation of carbonyl compds. with propanol in presence of ruthenium(II) complex catalysts and ephedrine-type ligands)
RN 64624-87-9 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)-, methyl ester (CA INDEX NAME)



REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 10 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:155152 HCAPLUS Full-text
DOCUMENT NUMBER: 135:5495
TITLE: Stereoselective synthesis of 3-substituted phthalides

via asymmetric transfer-hydrogenation using well-defined ruthenium catalysts under neutral conditions

AUTHOR(S): Everaere, K.; Scheffler, J.-L.; Mortreux, A.; Carpentier, J.-F.

CORPORATE SOURCE: Groupe de Chimie Organique Appliquee, Laboratoire de Catalyse de Lille Associe au CNRS, Ecole Nationale Superieure de Chimie de Lille, Villeneuve d'Ascq, Fr.

SOURCE: Tetrahedron Letters (2001), 42(10), 1899-1901
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

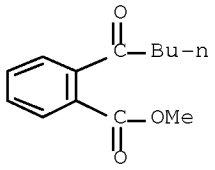
OTHER SOURCE(S): CASREACT 135:5495

AB The asym. transfer-hydrogenation of Me 2-acylbenzoates and iso-Pr 3-acetylpyridine-2-carboxylate in 2-propanol, in the absence of base, with preformed Ru diamido or alkoxy-amido complex catalysts provides 3-alkylphthalides in high yields and 92-97% ee. The procedure is, however, not as efficient for the preparation of optically active 3-phenylphthalide.

IT 64624-87-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of phthalides via asym. transfer-hydrogenation with ruthenium catalysts under neutral conditions)

RN 64624-87-9 HCAPLUS

CN Benzoic acid, 2-(1-oxopentyl)-, methyl ester (CA INDEX NAME)



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 11 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:655809 HCAPLUS Full-text

DOCUMENT NUMBER: 131:272001

TITLE: Method of storing active zero valent zinc metal and applications in organic synthesis

INVENTOR(S): Rieke, Reuben D.

PATENT ASSIGNEE(S): Board of Regents of the University of Nebraska, USA

SOURCE: U.S., 33 pp., Cont.-in-part of U.S. Ser. No. 917,587, abandoned.
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

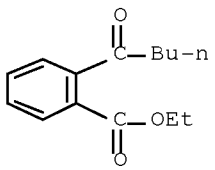
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5964919	A	19991012	US 1995-432828	19950502
US 5358546	A	19941025	US 1992-830629	19920204

US 5756653 A 19980526 US 1995-432995 19950502
PRIORITY APPLN. INFO.: US 1992-830629 A2 19920204
US 1992-917587 B2 19920721

AB There is claimed a method of storing an active zerovalent Zn metal consisting of: (a) suspending in a container the active Zn in an ethereal, hydrocarbon, aromatic hydrocarbon or aprotic polar solvent at a temperature of between -20° to 30° under an inert atmospheric; and (b) sealing the container; wherein the active Zn is stored for six months without substantial loss of activity. An object of the invention (not claimed) is to produce a Zn species that is more reactive than those obtained from traditional methods. The zerovalent Zn species is directly produced by reaction of a reducing agent on a Zn salt, preferably Zn(CN)2. Another object of the invention (not claimed) is to produce a Zn species that is highly reactive towards oxidative addition The organozinc reagent results from the reaction of the zerovalent Zn species and an organic compound having one or more stable anionic leaving groups. Yet another object of the invention (not claimed) is the direct production of a wide variety of organozinc compds., e.g., aryl, heterocyclic, arylalkyl, and polymeric Zn reagents that can undergo a number of valuable synthetic reactions. Still another object of the invention (not claimed) is to produce a wide variety of organozinc reagents that contain a broad spectrum of functional groups such as esters, ketones, nitrites, halides, amides, carbamates, epoxides, aldehydes, α,β-unsatd. enones (e.g., esters and. ketones), sulfoxides, sulfones, etc. Furthermore, an object of the invention (not claimed) is the synthesis of new organic compds. or the synthesis of known organic compds. using more effective and/or more direct synthetic methods. Many examples of copper-mediated reactions of organozinc halides with acid chlorides, α,β-unsatd. ketones, allylic halides, YCH2C.tplbond.CCH2Y (Y = Cl, OTs), and H2C:CBrCH2Br and palladium-catalyzed reactions with acid chlorides and aryl and vinyl halides are given. Also, the use of highly reactive Zn in the preparation of polythiophenes and poly-para-phenylene is illustrated; the 1st reported 3-alkylpolythiophene that is >99% regioregular is included. The examples are the same as in an earlier patent (WO 93/15086; Chemical Abstrs. accession number 120:54698).

IT 131379-20-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(method of storing active zero valent zinc metal and applications in organic synthesis)

RN 131379-20-9 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)-, ethyl ester (CA INDEX NAME)



REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

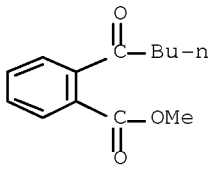
L28 ANSWER 12 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1998:343348 HCAPLUS Full-text
DOCUMENT NUMBER: 129:113627
ORIGINAL REFERENCE NO.: 129:23223a,23226a

TITLE: Liquid chromatographic-electrospray mass spectrometric study of the phthalides of Angelica sinensis and chemical changes of Z-ligustilide
AUTHOR(S): Lin, Long-Ze; He, Xian-Guo; Lian, Li-Zhi; King, Wayne; Elliott, Jerry
CORPORATE SOURCE: Research Laboratory of Natural Products Chemistry, East Earth Herb Inc., 4091 W. 11th Avenue, Eugene, OR, 97402, USA
SOURCE: Journal of Chromatography, A (1998), 810(1 + 2), 71-79
CODEN: JCRAEY; ISSN: 0021-9673
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB High-performance liquid chromatog.-electrospray ionization-mass spectrometry has been applied to analyze the chemical constituents of Danggui (the rhizome of Angelica sinensis) and to study chemical changes of Z-ligustilide. Twelve phthalides were unambiguously identified as senkyunolide I (3), senkyunolide H (4), sedanenolide (8), butylphthalide (9), E-ligustilide (13), Z-ligustilide (14), Z-butylidenephthalide (15), Z,Z'-6.8',7.3'- diligustilide (16), angelicide (17), levistolide A (18), Z-ligustilide dimer E-232 (19) and Z,Z'-3.3',8.8'-diligustilide (20) in Danggui extract The existence of 12 other phthalides (2, 5-7, 11, 12, 22-27), ferulic acid (1) and coniferyl ferulate (10) in Danggui extract has also been demonstrated. Phthalides 3, 4, 16-18 and 20 were determined to be the products from chemical change of Z-ligustilide. This is the first report of the existence of 16 compds. (2-8, 10-12, 20, 22-25 and 27) in Danggui extract

IT 64624-87-9
RL: ANT (Analyte); THU (Therapeutic use); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(liquid chromatog.-electrospray mass spectrometric study of the phthalides of Angelica sinensis and chemical changes of Z-ligustilide)

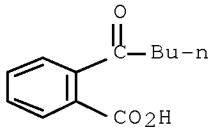
RN 64624-87-9 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)-, methyl ester (CA INDEX NAME)



REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 13 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1998:198830 HCAPLUS Full-text
DOCUMENT NUMBER: 128:316878
ORIGINAL REFERENCE NO.: 128:62621a,62624a
TITLE: Study on the metabolites of dl-3-n-butylphthalide in rats
AUTHOR(S): Wang, Chunhua; Feng, Yipu; Wu, Yuanliu
CORPORATE SOURCE: Institute of Materia Medica, Chinese Academy of Medical Science and Peking Union Medical College, Beijing, 100050, Peop. Rep. China
SOURCE: Yaoxue Xuebao (1997), 32(9), 641-646

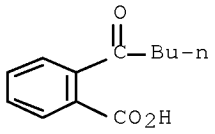
CODEN: YHHPAL; ISSN: 0513-4870
PUBLISHER: Chinese Academy of Medical Sciences, Institute of Materia Media
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB The metabolites of dl-3-n-butylphthalide (NBP) were studied in rats. Two main in vitro metabolites of NBP, M I and M II, were isolated and purified from rat liver microsome incubating system by using HPLC. Their structure was determined by spectral studies (UV, 1H- NMR, MS). Within 24 h following ig 3H-NBP, the total radioactivity excreted in urine and feces was 73.7% of the dose. Comparing with previous study, within 72 h following ig NBP, the total prototype drug excreted in urine and feces was 2.53% of the dose. This result excludes the possibility that NBP accumulates in vivo. The urine and brain homogenate of the rats (ig 3H-NBP) were analyzed by TLC. M I and M II were found in urine and M I was found in brain only. The ratio of radioactive M I to drug was 1 : 1 in rat brain within 1 h following ig 3H-NBP. The results suggest that M I might be an active metabolite.
IT 550-37-8
RL: BPR (Biological process); BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative); PROC (Process)
(study on the metabolites of dl-3-n-butylphthalide in rats)
RN 550-37-8 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)- (CA INDEX NAME)



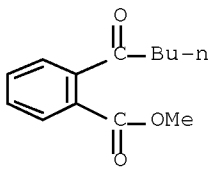
L28 ANSWER 14 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:804990 HCAPLUS Full-text
DOCUMENT NUMBER: 128:75228
ORIGINAL REFERENCE NO.: 128:14715a,14718a
TITLE: Microbial asymmetric syntheses of 3-alkylphthalide derivatives
AUTHOR(S): Kitayama, Takashi
CORPORATE SOURCE: Department of Agricultural Chemistry, Faculty of Agriculture, Kinki University, Nara, 631, Japan
SOURCE: Tetrahedron: Asymmetry (1997), 8(22), 3765-3774
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 128:75228
AB Phthalide derivs., almost all of which have an S-configuration, have a wide range of activity and exist in Angerica sinensis Diels and Sligusticum wallichiii Franch. For the first time, optically active (S)-3-methylphthalide derivs. were synthesized using two methods, asym. microbial reduction and microbial hydroxylation. For the first method, Me 2-acetylbenzoate was synthesized as a substrate, which was reduced asym. by Geotrichum candidum IFO 34614 to obtain (S)-3-methylphthalide in 92% yield (99% enantiomeric excess, ee). For the second method, 2-ethylbenzoic acid was employed as a substrate

which was hydroxylated asym. at the benzylic position by either Pseudomonas putida ATCC 12633 or Aspergillus niger IFO 6661, whose fermentation was induced by o-toluic acid, to obtain (S)-3-methylphthalide in 80% yield (99% ee). (S)-3-Butylphthalide and (S)-3-octylphthalide were obtained in the same manner in 12% yield (ee=99%) and 10% yield (ee=99%), resp.

IT 550-37-8P, 2-Pentanoylbenzoic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(microbial asym. syntheses of 3-alkylphthalide derivs.)
RN 550-37-8 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)- (CA INDEX NAME)



IT 64624-87-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(microbial asym. syntheses of 3-alkylphthalide derivs.)
RN 64624-87-9 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)-, methyl ester (CA INDEX NAME)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 15 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:766493 HCAPLUS Full-text
DOCUMENT NUMBER: 128:3590
ORIGINAL REFERENCE NO.: 128:779a,782a
TITLE: Synthesis of (Z)-3-butylidene-4,5-dihydroxyphthalide
AUTHOR(S): Li, Shaobai; Yan, Fulin; Wang, Zhiwei; Li, Yulin
CORPORATE SOURCE: State Key Laboratory of Applied Organic Chemistry, Institute of Organic Chemistry, Lanzhou University, Lanzhou, 730000, Peop. Rep. China
SOURCE: Huaxue Yanjiu Yu Yingyong (1997), 9(4), 338-342
CODEN: HYYIFM; ISSN: 1004-1656
PUBLISHER: Huaxue Yanjiu Yu Yingyong Bianjibu
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

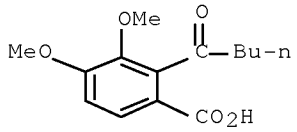
AB (Z)-3-Butylidenephthalide (I) and its derivs. were isolated as the Umbelliferae which are used frequently as an ingredient in the prescriptions of traditional Chinese medicine. (Z)-3-butylidene-4,5- dihydroxyphthalide

(II), an inhibitor of prostaglandin F2α, is a similar to I. II was prepared starting from 3,4-dimethoxybenzyl alc. or 3,4-methyldenedioxybenzyl alc. employing heteroatom directed lithiation reaction on aromatic compound

IT 198754-73-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of (Z)-3-butylidene-4,5-dihydroxyphthalide)

RN 198754-73-3 HCAPLUS

CN Benzoic acid, 3,4-dimethoxy-2-(1-oxopentyl)- (CA INDEX NAME)



L28 ANSWER 16 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:423919 HCAPLUS Full-text

DOCUMENT NUMBER: 125:137014

ORIGINAL REFERENCE NO.: 125:25537a,25540a

TITLE: Depsidone chemical transformations in an extract of the lichen Stereocaulon azoreum

AUTHOR(S): Gonzalez, Antonio G.; Rodriguez, Elsa M.; Bermejo, Jaime

CORPORATE SOURCE: Centro Productos Naturales Organicos, La Laguna, 38206, Spain

SOURCE: Anales de Quimica (1995), 91(5-6), 461-466
CODEN: ANQUEX; ISSN: 1130-2283

PUBLISHER: Real Sociedad Espanola de Quimica

DOCUMENT TYPE: Journal

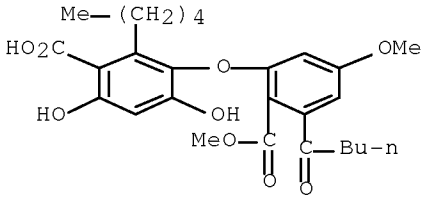
LANGUAGE: English

AB If the crude residue of an acetone extract of Stereocaulon azoreum was redissolved in a hexane:chloroform:methanol mixture and kept in the dark for three months, chemical transformations of stictic, cryptostictic and lobaric acids took place. The structures of the transformation products were established by mass spectrometry and 1H-13C-NMR spectral anal.

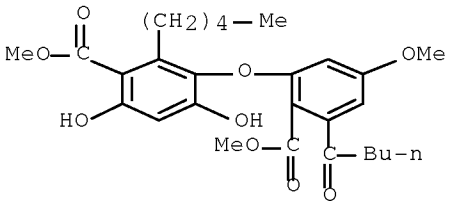
IT 179691-10-2 179691-11-3 179691-12-4
179691-13-5 179691-14-6
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); FMU (Formation, unclassified); PRP (Properties); BIOL (Biological study); FORM (Formation, nonpreparative); OCCU (Occurrence)
(depsidone chemical transformations in an extract of the lichen Stereocaulon
azoreum)

RN 179691-10-2 HCAPLUS

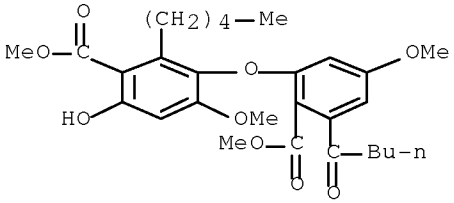
CN Benzoic acid, 4,6-dihydroxy-3-[5-methoxy-2-(methoxycarbonyl)-3-(1-oxopentyl)phenoxy]-2-pentyl- (CA INDEX NAME)



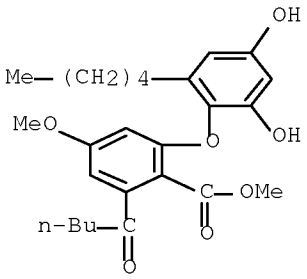
RN 179691-11-3 HCAPLUS
CN Benzoic acid, 4,6-dihydroxy-3-[5-methoxy-2-(methoxycarbonyl)-3-(1-oxopentyl)phenoxy]-2-pentyl-, methyl ester (CA INDEX NAME)



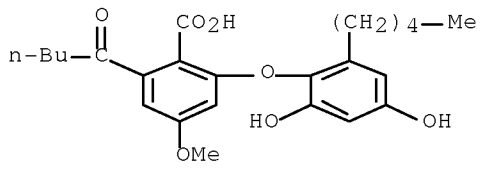
RN 179691-12-4 HCAPLUS
CN Benzoic acid, 6-hydroxy-4-methoxy-3-[5-methoxy-2-(methoxycarbonyl)-3-(1-oxopentyl)phenoxy]-2-pentyl-, methyl ester (CA INDEX NAME)



RN 179691-13-5 HCAPLUS
CN Benzoic acid, 2-(2,4-dihydroxy-6-pentylphenoxy)-4-methoxy-6-(1-oxopentyl)-, methyl ester (CA INDEX NAME)



RN 179691-14-6 HCAPLUS
CN Benzoic acid, 2-(2,4-dihydroxy-6-pentylphenoxy)-4-methoxy-6-(1-oxopentyl)- (CA INDEX NAME)

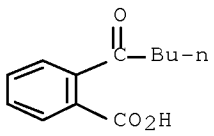


L28 ANSWER 17 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1996:198474 HCAPLUS Full-text
DOCUMENT NUMBER: 124:343016
ORIGINAL REFERENCE NO.: 124:63707a,63710a
TITLE: Efficient general asymmetric syntheses of 3-substituted 1(3H)-isobenzofuranones in very high enantiomeric excess
AUTHOR(S): Ramachandran, P. Veeraraghavan; Chen, Guang-Ming; Brown, Herbert C.
CORPORATE SOURCE: H.C. Brown and R. B. Wetherill Lab. Chem., Purdue Univ., West Lafayette, IN, 47907-1393, USA
SOURCE: Tetrahedron Letters (1996), 37(13), 2205-8
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:343016

AB The intermol. asym. reduction of Me o-(1-oxoalkyl)benzoates with β-chlorodiisopinocampheylborane provides, after workup, 3-alkylphthalides in ≥97% ee. Unfortunately, this procedure is not as efficient for the preparation of 3-arylphthalides. However, an intramol. reduction of B-(o-benzoylbenzoyloxy)diisopinocampheylborane, readily prepared by the treatment of o-benzyl benzoic acid with diisopinocampheylborane, provides 3-phenylphthalide in ≥96% ee.

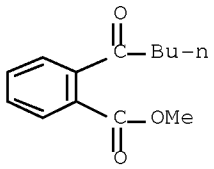
IT 550-37-8, Benzoic acid, 2-(1-oxopentyl)- 64624-87-9, Benzoic acid, 2-(1-oxopentyl)-, methyl ester
RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. syntheses of 3-substituted 1(3H)-isobenzofuranones)

RN 550-37-8 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)- (CA INDEX NAME)



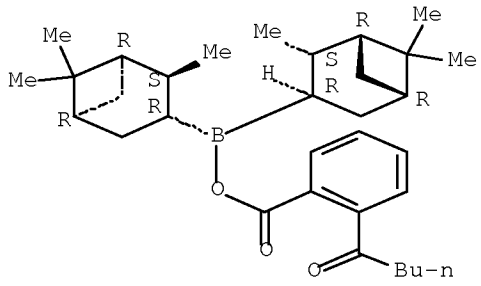
RN 64624-87-9 HCAPLUS

CN Benzoic acid, 2-(1-oxopentyl)-, methyl ester (CA INDEX NAME)



IT 176723-41-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(asym. syntheses of 3-substituted 1(3H)-isobenzofuranones)
RN 176723-41-4 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)-, anhydride with bis(2,6,6-trimethylbicyclo[3.1.1]hept-3-yl)borinic acid, [1R-[1α,2β,3α(1R*,2S*,3R*,5R*),5α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

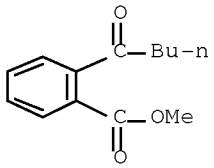


L28 ANSWER 18 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1995:837200 HCAPLUS Full-text
DOCUMENT NUMBER: 123:313625
ORIGINAL REFERENCE NO.: 123:56215a,56218a
TITLE: Syntheses of ligustilide and (±)-sedanenolide
AUTHOR(S): Li, Shao-Bai; Zhang, Shao-Ming; Li, Yu-Lin
CORPORATE SOURCE: Inst. of Organic Chemistry, Lanzhou Univ., Lanzhou, 730000, Peop. Rep. China
SOURCE: Gaodeng Xuexiao Huaxue Xuebao (1995), 16(9), 1420-2
CODEN: KTHPDM; ISSN: 0251-0790
PUBLISHER: Gaodeng Jiaoyu Chubanshe
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
OTHER SOURCE(S): CASREACT 123:313625
AB Z-ligustilide and sedanenolide are important naturally 3-alkylphthalide analogs occurring in many plants belonging to the Umbelliferae. They have antispasmodic antiasthmatic and smooth muscle relaxing activities. Herein the synthesis of (±)-sedanenolide is described, starting from phthalic anhydride as starting material. The key step in the synthesis is the Birch reduction of

3(Z)-butylidenephthalide, 3-methoxy-3-butylphthalide and Me o-valerylbenzoate. The yield in this step is 44%-60%. The synthesis of ligustilide was studied.

IT 64624-87-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(syntheses of ligustilide and (±)-sedanenolide via Birch reduction)

RN 64624-87-9 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)-, methyl ester (CA INDEX NAME)



L28 ANSWER 19 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1995:742952 HCAPLUS Full-text
DOCUMENT NUMBER: 123:143629
ORIGINAL REFERENCE NO.: 123:25577a,25580a
TITLE: Preparation of 4,5-dihydro-3-(hydroxy)alkyl phthalides
INVENTOR(S): Li, Shaobai; Zhang, Shaoming; Li, Yulin
PATENT ASSIGNEE(S): Lanzhou University, Peop. Rep. China
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 5 pp.
CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

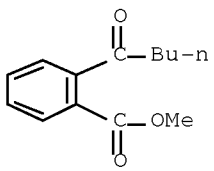
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1087633	A	19940608	CN 1992-111279	19920930
CN 1034808	C	19970507		

PRIORITY APPLN. INFO.: CN 1992-111279 19920930

AB Title compds. were prepared by Birch reduction of o-acylbenzoates or 3-alkyl(idene)phthalides optionally substituted with a hydroxyl or carbonyl group on the alkyl(idene) group in liquid ammonia or amine by Na, Li, or K.

IT 64624-87-9, Methyl 2-valerylbenzoate
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 4,5-dihydro-3-(hydroxy)alkyl phthalides)

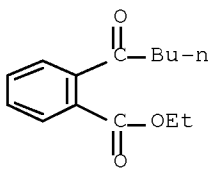
RN 64624-87-9 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)-, methyl ester (CA INDEX NAME)



L28 ANSWER 20 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1994:54698 HCAPLUS Full-text
DOCUMENT NUMBER: 120:54698
ORIGINAL REFERENCE NO.: 120:9991a,9994a
TITLE: Preparation of highly reactive forms of zinc and reagents therefrom
INVENTOR(S): Rieke, Rueben D.
PATENT ASSIGNEE(S): University of Nebraska, USA
SOURCE: PCT Int. Appl., 122 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9315086	A1	19930805	WO 1992-US8542	19921007
W: AT, AU, BB, BG, BR, CA, CH, CS, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MG, MN, MW, NL, NO, PL, RO, RU, SD, SE				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG				
US 5358546	A	19941025	US 1992-830629	19920204
AU 9227878	A	19930901	AU 1992-27878	19921007
US 5756653	A	19980526	US 1995-432995	19950502
PRIORITY APPLN. INFO.:			US 1992-830629 A	19920204
			US 1992-917587 A	19920721
			WO 1992-US8542 A	19921007

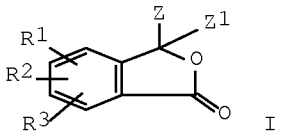
OTHER SOURCE(S): CASREACT 120:54698
AB The preparation of novel zerovalent zinc species and organozinc reagents are described. The zerovalent zinc species is directly produced by action of a reducing agent on a zinc salt, preferably Zn(CN)2. The organozinc reagent is prepared by reaction of the zerovalent zinc species and an organic compound having one or more stable anionic leaving groups. These organozinc reagents include a wide spectrum of functional groups in the organic radical, and are useful in a variety of reaction schemes. Thus, reaction of Zn(CN)2 with lithium in the presence of naphthalene in THF gave highly reactive Zn metal which on treatment with 4-BrC6H4Me gave 100% 4-MeC6H4ZnBr (I). The reaction of I with various organic halides are described.
IT 131379-20-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 131379-20-9 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)-, ethyl ester (CA INDEX NAME)



L28 ANSWER 21 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1992:469721 HCAPLUS Full-text
DOCUMENT NUMBER: 117:69721
ORIGINAL REFERENCE NO.: 117:12259a,12262a
TITLE: Preparation of phthalide derivatives as prostaglandin F2α inhibitors
INVENTOR(S): Ogawa, Yoshimitsu; Hosaka, Kunio; Kubota, Kiyoshi; Chin, Masao
PATENT ASSIGNEE(S): Tsumura K. K., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 25 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04077480	A	19920311	JP 1990-189436	19900719

PRIORITY APPLN. INFO.: JP 1990-189436 19900719
OTHER SOURCE(S): MARPAT 117:69721
GI

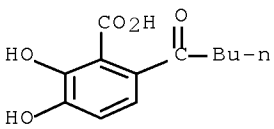


I

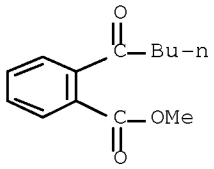
AB The title compds. (I; Z = Bu; Z1 = H, OH; or ZZ1 = CHPr; R1-R3 = MeO, OH, H) are prepared Thus, metalation of 6,7-dimethoxyphthalide (preparation given) with 1.6 M BuLi in (Me2CH)2NH/THF followed by a solution of ZnCl2 in THF AT -40° and reaction with a solution of n-butyraldehyde at -40° gave 77.8 % 3-(1-hydroxybutyl)-6,7-dimethoxyphthalide. Mesylation of this with MeSO2Cl in pyridine/benzene under reflux and treatment of the resulting 3-(1-mesyloxybutyl)-6,7-dimethoxyphthalide with DBU in refluxing benzene gave 22 % (Z)- and (E)-3-butylidene-6,7-dimethoxyphthalide. (Z)-3-Butylidene-5,6-dihydroxyphthalide at 5 × 10-6 g/mL in vitro inhibited 50.7 ± 7.3% prostaglandin F2α. A total of 27 I were prepared

IT 138350-82-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as prostaglandin F2α inhibitor)

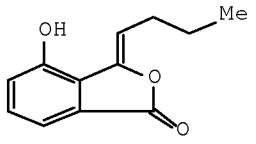
RN 138350-82-0 HCAPLUS
CN Benzoic acid, 2,3-dihydroxy-6-(1-oxopentyl)- (CA INDEX NAME)



L28 ANSWER 22 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1992:444606 HCAPLUS Full-text
DOCUMENT NUMBER: 117:44606
ORIGINAL REFERENCE NO.: 117:7855a,7858a
TITLE: A phthalide and 2-farnesyl-6-methyl benzoquinone from Ligusticum chuanxiong
AUTHOR(S): Naito, Takashi; Niitsu, Kazuaki; Ikeya, Yukinobu; Okada, Minoru; Mitsuhashi, Hiroshi
CORPORATE SOURCE: Res. Inst. Biol. Chem., Tsumura and Co., Ibaraki, 300-11, Japan
SOURCE: Phytochemistry (1992), 31(5), 1787-9
CODEN: PYTCAS; ISSN: 0031-9422
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A new phthalide, senkyunolide Q, and 2-farnesyl-6-Me benzoquinone, senkyunone, along with senkyunolide M, 2-methoxy-4-(3-methoxy-1-propenyl)- phenol, and 2-(1-oxo-pentyl)-benzoic acid Me ester were isolated from the rhizome of Ligusticum chuangxiong. On the basis of spectral analyses and chemical methods, the structures of senkyunolide Q and senkyunone were proven to be (6RS,7SR)-3-butylidene-4,5,6,7-tetrahydro-7-hydroxy-6-(1-oxobutyl)- phthalide and (2'E,6'E)-2-farnesyl-6-methyl-p-benzoquinone, resp.
IT 64624-87-9
RL: BIOL (Biological study)
(from Ligusticum chuangxiong)
RN 64624-87-9 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)-, methyl ester (CA INDEX NAME)



L28 ANSWER 23 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1992:128551 HCAPLUS Full-text
DOCUMENT NUMBER: 116:128551
ORIGINAL REFERENCE NO.: 116:21755a,21758a
TITLE: Synthesis of (Z)-3-butylidene-4-hydroxyphthalide
AUTHOR(S): Ogawa, Y.; Hosaka, K.; Chin, M.; Mitsuhashi, H.
CORPORATE SOURCE: Res. Inst. Biol. Chem., Tsumura and Co., Ami, 300-11, Japan
SOURCE: Synthetic Communications (1992), 22(2), 315-21
CODEN: SYNCAV; ISSN: 0039-7911
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 116:128551
GI



I

AB (Z)-3-Butylidene-4-hydroxyphthalide (I) was synthesized regio- and stereoselectively from 3-methoxybenzyl alc. in 4 steps involving regioselective lithiation and alkylation with BuCHO, oxidation with Bu4N+MnO4-, intramol. cyclization in presence of SOCl2, and O-demethylation.

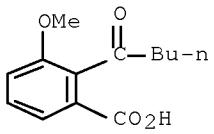
IT 116541-39-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and intramol. cyclization of, in presence of thionyl chloride)

RN 116541-39-0 HCAPLUS

CN Benzoic acid, 3-methoxy-2-(1-oxopentyl)- (CA INDEX NAME)



L28 ANSWER 24 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1992:41224 HCAPLUS Full-text

DOCUMENT NUMBER: 116:41224

ORIGINAL REFERENCE NO.: 116:7065a,7068a

TITLE: Synthesis of (Z)-3-butylidene-6,7-dihydroxyphthalide

AUTHOR(S): Ogawa, Yoshimitsu; Hosaka, Kunio; Chin, Masao; Mitsuhashi, Hiroshi

CORPORATE SOURCE: Res. Inst. Biol. Chem., Tsumura and Co., Ibaraki, 300-11, Japan

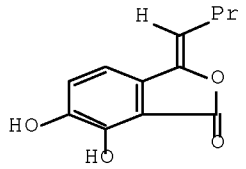
SOURCE: Heterocycles (1991), 32(9), 1737-44
CODEN: HTCYAM; ISSN: 0385-5414

DOCUMENT TYPE: Journal

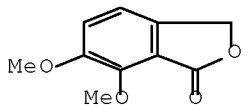
LANGUAGE: English

OTHER SOURCE(S): CASREACT 116:41224

GI



I



II

AB The title compound I was first synthesized from dimethoxyphthalide II in 3 steps and its structure was synthetically confirmed.

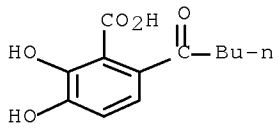
IT 138350-82-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and cyclization of)

RN 138350-82-0 HCAPLUS

CN Benzoic acid, 2,3-dihydroxy-6-(1-oxopentyl)- (CA INDEX NAME)



L28 ANSWER 25 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1991:81102 HCAPLUS Full-text

DOCUMENT NUMBER: 114:81102

ORIGINAL REFERENCE NO.: 114:13829a,13832a

TITLE: The direct formation of functionalized alkyl(aryl)zinc halides by oxidative addition of highly reactive zinc with organic halides and their reactions with acid chlorides, α,β-unsaturated ketones, and allylic, aryl, and vinyl halides

AUTHOR(S): Zhu, Lishan; Wehmeyer, Richard M.; Rieke, Reuben D.

CORPORATE SOURCE: Dep. Chem., Univ. Nebraska-Lincoln, Lincoln, NE, 68588-0304, USA

SOURCE: Journal of Organic Chemistry (1991), 56(4), 1445-53
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 114:81102

AB Highly reactive zinc, prepared by reduction of ZnCl2 with lithium naphthalenide, readily undergoes oxidative addition to alkyl, aryl, and vinyl halides under mild conditions to generate the corresponding organozinc compds. in excellent yields. Significantly, the reaction will tolerate a spectrum of functional groups on the organic halides. Accordingly, this approach can now be used to prepare a wide variety of highly functionalized organozinc compds. In the presence of Cu(I) salts, the organozinc compds. cross-couple with acid chlorides, conjugatively add to α,β-unsatd. ketones, and regioselectively undergo SN2' substitution reactions with allylic halides. They also cross-couple with aryl or vinyl halides with Pd(0) catalysts.

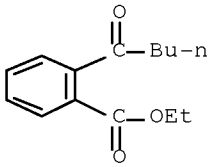
IT 131379-20-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 131379-20-9 HCAPLUS

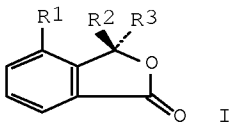
CN Benzoic acid, 2-(1-oxopentyl)-, ethyl ester (CA INDEX NAME)



L28 ANSWER 26 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1990:98368 HCAPLUS Full-text
DOCUMENT NUMBER: 112:98368
ORIGINAL REFERENCE NO.: 112:16727a,16730a
TITLE: Phthalides as prostaglandin F 2α inhibitors and their preparation
INVENTOR(S): Ogawa, Yoshimitsu; Chin, Masao; Hosaka, Kunio; Kubota, Kiyoshi
PATENT ASSIGNEE(S): Tsumura and Co., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 01199958	A	19890811	JP 1987-182228	19870723

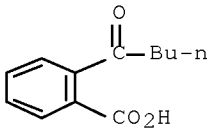
PRIORITY APPLN. INFO.: JP 1987-182228 19870723
OTHER SOURCE(S): MARPAT 112:98368
GI



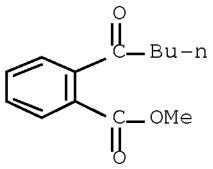
I

AB The title compds. I (R1 = H, MeO; when R2 is Bu, R3 is H, or when R2 is H, R3 = Bu; excluding the case where R1 = R2 = H and R3 = Bu), useful as prostaglandin F 2α inhibitors, were prepared A mixture of (-)-3-butyl-1-hydroxy-4-methoxy-2-oxaindan, AgNO3, and NaOH in MeOH-H2O was stirred at room temperature for 1 h to give (-)-4-methoxy-3-butylphthalide (II). II in vitro inhibited prostaglandin F 2α by 29.7%.

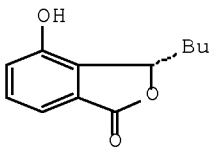
IT 550-37-8P 64624-87-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of prostaglandin F 2α inhibitor)
RN 550-37-8 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)- (CA INDEX NAME)



RN 64624-87-9 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)-, methyl ester (CA INDEX NAME)

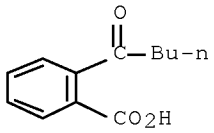


L28 ANSWER 27 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1990:76773 HCAPLUS Full-text
DOCUMENT NUMBER: 112:76773
ORIGINAL REFERENCE NO.: 112:13115a,13118a
TITLE: Synthesis of (-)-3-butyl-4-hydroxyphthalide
AUTHOR(S): Ogawa, Yoshimitsu; Hosaka, Kunio; Chin, Masao; Mitsuhashi, Hiroshi
CORPORATE SOURCE: Res. Inst. Biol. Chem., Tsumura and Co., Ami, 300-11, Japan
SOURCE: Heterocycles (1989), 29(5), 865-72
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:76773
GI

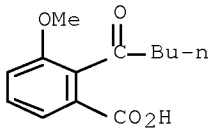


I

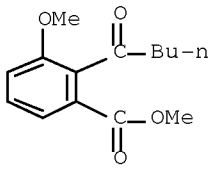
AB (-)-3-Butyl-4-hydroxyphthalide (I) was synthesized enantioselectively and its absolute stereochem. at C-3 was determined to be S.
IT 550-37-8, 2-Valerylbenzoic acid 116541-39-0, 3-Methoxy-2-valerylbenzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification of)
RN 550-37-8 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)- (CA INDEX NAME)



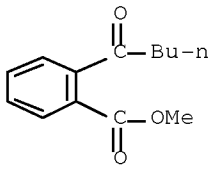
RN 116541-39-0 HCAPLUS
CN Benzoic acid, 3-methoxy-2-(1-oxopentyl)- (CA INDEX NAME)



IT 124831-72-7P, Methyl 3-methoxy-2-valerylbenzoate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and attempted reduction of)
RN 124831-72-7 HCAPLUS
CN Benzoic acid, 3-methoxy-2-(1-oxopentyl)-, methyl ester (CA INDEX NAME)



IT 64624-87-9P, Methyl 2-valerylbenzoate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
RN 64624-87-9 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)-, methyl ester (CA INDEX NAME)

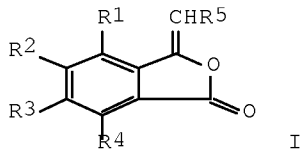


L28 ANSWER 28 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1988:528817 HCAPLUS Full-text
DOCUMENT NUMBER: 109:128817
ORIGINAL REFERENCE NO.: 109:21457a,21460a
TITLE: Preparation of phthalide derivatives as prostaglandin F2α inhibitors
INVENTOR(S): Ogawa, Yoshimitsu; Chin, Masao; Hosaka, Kunio; Kubota, Kiyoshi
PATENT ASSIGNEE(S): Tsumura Juntendo, Inc., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 26 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63083081	A	19880413	JP 1986-228264	19860929
JP 07108906	B	19951122		

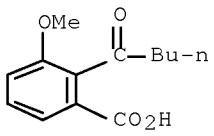
PRIORITY APPLN. INFO.: JP 1986-228264 19860929
OTHER SOURCE(S): MARPAT 109:128817
GI



I

AB The title compds. [I; R1 = H, OH, OMe, NO2; R2 = H, OH, OMe, OCH2OMe; R3 = H, OMe; R4 = H, NO2; R5 = H, alkyl, (CH2)3CO2H, (CH2)3CO2Et, (CH2)4OH], useful as prostaglandin F2α inhibitors, are prepared Cycloamidation of 3,4-(MeO)2C6H3CO2Cl with 2-amino-2-methyl-4-propanol and then treatment of the resultant amide with SOCl2 gave 83% 2-(3,4-dimethoxyphenyl)-4,4-dimethyloxazoline which was reacted with BuLi and then paraformaldehyde at -45° to give 77% 4,5-dimethoxyphthalide (II). Reaction of II with n-PrCHO in the presence of n-BuLi, (Me2CH)2NH, and ZnCl2 in THF at -40° overnight gave 97% 4,5-dimethoxy-3-(1-hydroxybutyl)-phthalide which in C6H6 was refluxed with MeClSO2 in the presence of pyridine to give 99% 4,5-dimethoxy-3-(1-methanesulfonyloxybutyl)phthalide and the elimination reaction of the latter by refluxing in the presence of 1,8-diazabicyclo[5.4.0]undec-7-ene in C6H6 to give 74% (Z)- and 4.0% (E)-I (R1 = R2 = OMe, R3 = R4 = H, R5 = Pr). Also, (Z)-I (R1 = OH, R2-R4 = H, R5 = Pr) at 5 × 10-8 g/mL in EtOH showed 48% inhibition of rat uterus contraction generated by prostaglandin F2α.

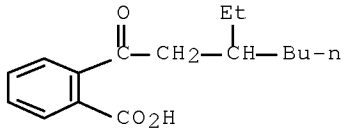
IT 116541-39-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclocondensation of)
RN 116541-39-0 HCAPLUS
CN Benzoic acid, 3-methoxy-2-(1-oxopentyl)- (CA INDEX NAME)



L28 ANSWER 29 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1987:62796 HCAPLUS Full-text
DOCUMENT NUMBER: 106:62796
ORIGINAL REFERENCE NO.: 106:10271a
TITLE: Mitogenicity of peroxisome proliferators in monolayers of adult rat hepatocytes
AUTHOR(S): Bieri, F.; Bentley, P.; Waechter, F.; Staeubli, W.
CORPORATE SOURCE: Cent. Toxicol. Unit, Ciba-Geigy Ltd., Basel, 4002, Switz.
SOURCE: Food and Chemical Toxicology (1986), 24(6-7), 709
CODEN: FCTOD7; ISSN: 0278-6915
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The induction of peroxisomal enzymes and of replicative DNA synthesis were studied to examine the possible interrelation between these effects and to classify their importance in the carcinogenic process. The time course and reversibility of both effects were superimposable, but the dose response differed, being linear ≤100 μg/mL for peroxisomal enzyme induction, and showing a maximum at 10 μg/mL for induction of DNA synthesis. Several substances (e.g., prostaglandin synthesis inhibitors and antioxidants) were added to the culture medium to alter either replicative DNA synthesis or the oxidative effects resulting from peroxisome proliferation. The 2 parameters seemed to be altered independently, providing no evidence of any direct correlation. Dose-response curves with known peroxisome proliferators and related compds. indicated that the mitogenic potency of the proliferators could not be predicted from their effects on the peroxisomal compartment. Ranking of the substances according to their ability to induce replicative DNA synthesis in cultured hepatocytes was more in agreement with their hepatomegalic potency than was their ranking as peroxisome proliferators. The mitogenic potency of the substance and the peroxisome proliferation should be measured when the monolayers of adult rat hepatocytes are used to assess the possible hepatocarcinogenicity of the test substances.

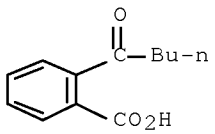
IT 106462-12-8
RL: BIOL (Biological study)
(peroxisome proliferator, mitogenicity of, in hepatocytes, hepatocarcinogenesis in relation to)
RN 106462-12-8 HCAPLUS
CN Benzoic acid, 2-(3-ethyl-1-oxoheptyl)- (CA INDEX NAME)



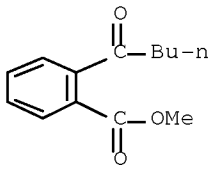
L28 ANSWER 30 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1981:602924 HCAPLUS Full-text
DOCUMENT NUMBER: 95:202924
ORIGINAL REFERENCE NO.: 95:33897a,33900a
TITLE: Deactivation of triplet phenyl alkyl ketones by conjugatively electron-withdrawing substituents
AUTHOR(S): Wagner, Peter J.; Siebert, Elizabeth J.
CORPORATE SOURCE: Dep. Chem., Michigan State Univ., East Lansing, MI, 48824, USA
SOURCE: Journal of the American Chemical Society (1981), 103(24), 7329-35
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Cyano, carbomethoxy and acyl para substituents decrease the triplet reactivity of PhCOBu (γ-H abstraction); comparable meta substituents increase reactivity. Spectroscopic results indicate that para (-R) substituents lower π,π* triplet energies so much more than n,π* energies that the lowest triplets become largely π,π* in nature. Meta (-R) substituents do not stabilize π,π* triplets enough to invert triplet levels. Both substitution patterns support a largely 1,4-biradical structure for the lowest π,π* triplet of acylbenzenes. Ortho substituents show the usual steric anomalies. An o-cyano group enhanced PhCOBu triplet reactivity by stabilizing the n,π* triplet; o-carbomethoxy deactivates PhCOBu by stabilizing the π,π* triplet but not the n,π*.

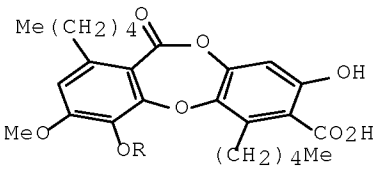
IT 550-37-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of)
RN 550-37-8 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)- (CA INDEX NAME)



IT 64624-87-9
RL: PRP (Properties)
(triplet reactivity of)
RN 64624-87-9 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)-, methyl ester (CA INDEX NAME)

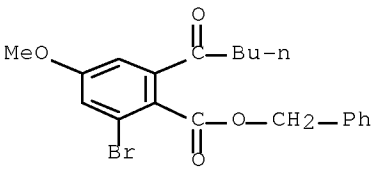


L28 ANSWER 31 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1977:601488 HCAPLUS Full-text
DOCUMENT NUMBER: 87:201488
ORIGINAL REFERENCE NO.: 87:31903a,31906a
TITLE: Depsidone synthesis. X. Methoxy- and hydroxycolensoic acids
AUTHOR(S): Djura, Peter; Sargent, Melvyn V.; Clark, Paul D.
CORPORATE SOURCE: Dep. Org. Chem., Univ. West. Australia, Nedlands, Australia
SOURCE: Australian Journal of Chemistry (1977), 30(7), 1545-51
CODEN: AJCHAS; ISSN: 0004-9425
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



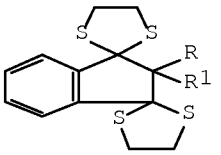
I, R=Me
II, R=H

AB The synthesis of the lichen depsidones methoxycolensoic acid (I) and hydroxycolensoic acid (II) is described. An attempt to synthesize depsidones of the lobaric acid-type is also reported.
IT 64750-36-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 64750-36-3 HCAPLUS
CN Benzoic acid, 2-bromo-4-methoxy-6-(1-oxopentyl)-, phenylmethyl ester (CA INDEX NAME)

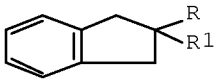


L28 ANSWER 32 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1977:601145 HCAPLUS Full-text
DOCUMENT NUMBER: 87:201145
ORIGINAL REFERENCE NO.: 87:31839a,31842a
TITLE: A novel synthesis of 2-substituted indans
AUTHOR(S): Mitra, R. B.; Kulkarni, G. H.; Khanna, P. N.

CORPORATE SOURCE: Natl. Chem. Lab., Poona, India
SOURCE: Synthesis (1977), (6), 415-17
CODEN: SYNTBF; ISSN: 0039-7881
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 87:201145
GI



I

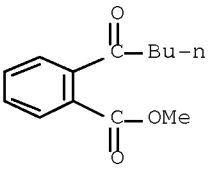


II

AB 1,3-Indandione bis-ketals I (R = H, Me, Et, Pr; R1 = H, Me) were desulfurized by Raney Ni in EtOH at reflux to give indans II. The intramol. cyclocondensation of 2-(RCHR1CO)C6H4CO2Me in the presence of HSCH2CH2SH gave I.

IT 64624-87-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(intramol. cyclocondensation of, and ketalization of product from)

RN 64624-87-9 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)-, methyl ester (CA INDEX NAME)



L28 ANSWER 33 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1976:577680 HCAPLUS Full-text
DOCUMENT NUMBER: 85:177680
ORIGINAL REFERENCE NO.: 85:28407a,28410a
TITLE: Synthetic studies on (2R,4'R,8'R)-α-tocopherol. Facile syntheses of optically active, saturated, acyclic isoprenoids via stereospecific [3,3] sigmatropic rearrangements
AUTHOR(S): Chan, Ka-Kong; Cohen, Noal; De Noble, James P.; Specian, Anthony C., Jr.; Saucy, Gabriel
CORPORATE SOURCE: Chem. Res. Dep., Hoffmann-La Roche, Inc., Nutley, NJ, USA
SOURCE: Journal of Organic Chemistry (1976), 41(22), 3497-505
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English

AB (+)-(R)-HO2CCH2CHMe(CH2)3CHMe2 was stereospecifically prepared from Me2CHCH2CHO via [3,3] sigmatropic rearrangements of (+)-(R)-(Z)- and (-)-(S)-(E)-MeCH:CHCH(OH)CH2CHMe2. Similarly, (+)-(R)- OCHCH2CHMe(CH2)3CHMe2 gave in very high optical purity (3S,7R)-EtO2CCH2CHMeCH:CHCH2CHMe(CH2)3CHMe2, which was converted into (3R,7R)-HOCH2CH2CHMe(CH2)3CHMe(CH2)3CHMe2, an intermediate in the synthesis of (2R,4'R,8'R)-α-tocopherol.

IT 59983-75-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenation of)

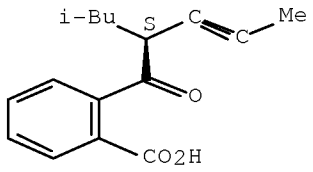
RN 59983-75-4 HCAPLUS

CN Benzoic acid, 2-[2-(2-methylpropyl)-1-oxo-3-pentynyl]-, (S)-, compd. with (S)-α-methylbenzenemethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 59983-74-3
CMF C16 H18 O3

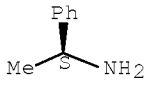
Absolute stereochemistry.



CM 2

CRN 2627-86-3
CMF C8 H11 N

Absolute stereochemistry. Rotation (-).



L28 ANSWER 34 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1976:58932 HCAPLUS Full-text
DOCUMENT NUMBER: 84:58932
ORIGINAL REFERENCE NO.: 84:9675a,9678a
TITLE: Keto acids
INVENTOR(S): Watanabe, Yoshihisa
PATENT ASSIGNEE(S): Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 3 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

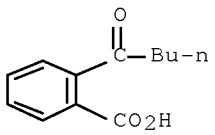
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 50112319	A	19750903	JP 1974-20448	19740222
PRIORITY APPLN. INFO.:			JP 1974-20448 A	19740222

AB Aliphatic or aromatic polycarboxylic acid anhydrides were treated with an iron carbonyl salt and then alkylated with an alkyl halide to give aliphatic or aromatic keto acids. Thus, 1.5 ml Fe(CO)5 in THF was added to Na-Hg (prepared from 0.7 g Na and 80 g Hg) in THF under Ar and Hg removed to give Na2Fe(CO)4. To this 1.14 g glutaric anhydride and 3.8 g BuI were added and the mixture was stirred 2 hr to give 1.32 g 5-oxononanoic acid. Similarly, succinic anhydride and BuI (MeI) gave 4-oxooctanoic acid (or 4-oxopentanoic acid); phthalic anhydride and BuI gave o-valerylbenzoic acid.

IT 550-37-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 550-37-8 HCAPLUS

CN Benzoic acid, 2-(1-oxopentyl)- (CA INDEX NAME)



L28 ANSWER 35 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1974:504920 HCAPLUS Full-text

DOCUMENT NUMBER: 81:104920

ORIGINAL REFERENCE NO.: 81:16583a,16586a

TITLE: Oxidative decyanation of arylacetonitriles. Synthesis of ligusticumic acid

AUTHOR(S): Watt, David S.

CORPORATE SOURCE: Dep. Chem., Univ. Colorado, Boulder, CO, USA

SOURCE: Journal of Organic Chemistry (1974), 39(18), 2799-2800
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

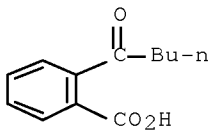
OTHER SOURCE(S): CASREACT 81:104920

AB The oxidative decyanation of arylacetonitriles ArCH(CN)R to ketones ArCOR was effected in three steps: silylation of ArC(Li)(CN)R with Me3CSiMe2Cl to afford Ar-CR:C:NSi(CMe3)Me2, iodination of the ketenimine to afford ArC(I)(CN)R, and Ag2O conversion of the α-iodo nitrile to ArCOR. The application of this methodology to the synthesis of ligusticumic acid is reported.

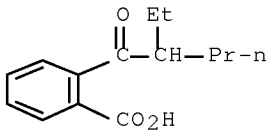
IT 550-37-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 550-37-8 HCAPLUS

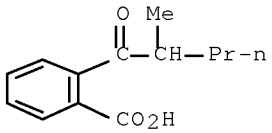
CN Benzoic acid, 2-(1-oxopentyl)- (CA INDEX NAME)



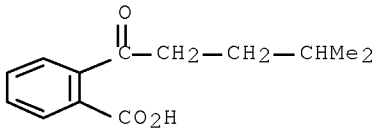
L28 ANSWER 36 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1964:411191 HCAPLUS Full-text
DOCUMENT NUMBER: 61:11191
ORIGINAL REFERENCE NO.: 61:1805f-h,1806e-f
TITLE: Alkylated indandiones with anticonvulsive activity
AUTHOR(S): Aebi, A.; Gyurech-Vago, E.; Hofstetter, E.; Waser, P.
CORPORATE SOURCE: CIBA Ltd., Basel, Switz.
SOURCE: Pharmaceutica Acta Helvetiae (1963), 38(7-8), 407-17
CODEN: PAHEAA; ISSN: 0031-6865
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB Alkylated indandiones with short side-chains exhibit anticonvulsive activity although they are inferior to earlier known anticonvulsives. Na (1.2 g.) in 40 ml. EtOH was heated 6 hrs. at 130-40° with 7.4 g. 2-methylindan-1,3-dione and 7 g. PrBr in a closed container to give 4.7 g. 2-methyl-2-propylindan-1,3-dione (I), m. 56-7° (EtOH). The following Ia were similarly prepared (R, R1, and m.p. or b.p. given): Me, H, (II) 86-7°; Et, H, 52-4°; Me, Me (III), 104-6°; Me, Et, 46-7°; Me, isoBu, b0.1 82-5°; Me, iso-Pr, b0.1 93-7°; Me, Bu, 41-3°; Me, Am, b0.5 120°; Me, n-C8H17, b10 153-6°; Et, Et, 15°; Et, Pr, b0.5 103-7°; Et, iso-Pr, b0.1 88-91°; Et, Bu, b0.1 105-8°; Et, isoBu, 61-3° (b0.1 104-9°); Pr, Pr, -; Bu, Bu, 71-2°; Ph, Me, 154-5°; Ph, Bu, b0.3 145-7°. Air oxiup. for 4 months at room temperature of 11 g. II gave 3.9 g. phthalic acid (IV), m. 199° (decomposition), and 0.5 g. 2-methyl-2-hydroxyindan-1,3-dione, m. 100-2° (stable indefinitely when stored under N). II (1.6 g.) in 10 ml. AcOH treated with 4 ml. 30% H2O2 overnight at room temperature and for an addnl. hr. at 40-50° gave 0.5 g. IV. II (1.6 g.) in 60 ml.N NaOH with 3 ml. 30% H2O2 0.5 hr. at 40° and overnight at room temperature gave 1.3 g. IV, which on heating to 200° gave phthalic anhydride, m. 127-9°. I (10 g.), 90 ml. 2N NaOH, and 60 ml. EtOH refluxed 18 hrs. gave 10 g. o-(2-methylvaleroyl)benzoic acid, b0.1 100°. The following o-RR1CHCOC6H4CO2H were similarly prepared (R, R1, and m.p. given): Me, Me (V), 119-21°; Me, Et, 95-7°; Me, Pr, -; Me, iso-Pr, 63-5°; Me, Bu, 45-7°; Et, Pr, -; Me, n-C8H17, 48-59°. 3-Isopropylidenephthalide, m. 93-4° (EtOH), was prepared from V by heating 2 hrs. at 200°, or by refluxing 1.9 g. V and 2 g. PCl5 in 100 ml. absolute EtOH 3 hrs. III (1.75 g.) in 70 ml. AcOH hydrogenated over PtO2 at 25° and 1 atmospheric gave 0.5 g. 2,2-dimethyl-3-hydroxyindan-1- one, m. 89-90° (aqueous EtOH). III (3.5 g.) in 50 g. AcOH similarly hydrogenated gave 1.5 g. 2,2-dimethyl-1,3-dihydroxyindan, m. 159-60° (Et2O). The ultraviolet spectra of some of the compds. were reported.
IT 92864-18-1P, Benzoic acid, o-(2-ethylvaleryl)- 97024-19-6P, Benzoic acid, o-(2-methylvaleryl)-
RL: PREP (Preparation)
(preparation of)
RN 92864-18-1 HCAPLUS
CN Benzoic acid, o-(2-ethylvaleryl)- (7CI) (CA INDEX NAME)



RN 97024-19-6 HCAPLUS
CN Benzoic acid, o-(2-methylvaleryl)- (7CI) (CA INDEX NAME)



L28 ANSWER 37 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1954:14622 HCAPLUS Full-text
DOCUMENT NUMBER: 48:14622
ORIGINAL REFERENCE NO.: 48:2661f-i
TITLE: Synthesis of alkylidenephthalides and their odor
AUTHOR(S): Kariyone, Tatsuo; Shimizu, Shuichi
CORPORATE SOURCE: Univ. Kyoto
SOURCE: Yakugaku Zasshi (1953), 73, 336-8
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB RMgX (6.1 g. Mg, 50 g. Me2CHCH2CH2Br, and 150 ml. dry Et2O) treated portionwise with 20 g. powdered CdCl2, heated 20 min., 17 g. o-C6H4(CO)2O in 100 ml. Et2O added with ice cooling, the mixture heated 1 hr., 10% H2SO4 added with ice cooling, the solution extracted with Et2O, the Et2O layer washed with 40 ml. 10% Na2CO3, the aqueous layer acidified with dilute H2SO4, and the oily layer distilled in vacuo give 15 g. o-HO2CC6H4COCH2CH2CHMe2 (I), b8 160°; I in 60 ml. 50% H2SO4 heated on a water bath 6-7 hrs., the product poured into cold water, and the oily product washed with 5% Na2CO3 and water then distilled in vacuo give o-C6H4.C(:R).O.CO (II) (R = CHCH2CHMe2), b7 170-2°. Other II: R = CH2, m. 58-60°; CHMe, m. 64°; CMe2, m. 96°; CHEt, b12 170°; CHCHMe2, m. 97°; CHPr, b6 134°; CHCH:CH2, b6 125-30°; CHPh (III), m. 96° (no aroma); CHC6H4Me-p (IV), m. 152°. 3-Butylidenetetrahydrophthalide (V), b7 140-2°. The aroma of the II increases with an increasing number of C atoms in R; II with R = Pr or Bu are most similar to Ligusticum acutilobum (VI); III and IV have an unpleasant odor, although the reduction of the C6H6 nucleus in the phthalide resulted in an aroma similar to that of VI.
IT 860698-74-4P, Benzoic acid, o-(4-methylvaleryl)-
RL: PREP (Preparation)
(preparation of)
RN 860698-74-4 HCAPLUS
CN Benzoic acid, 2-(4-methyl-1-oxopentyl)- (CA INDEX NAME)

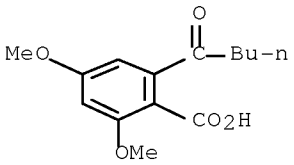


L28 ANSWER 38 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1941:30348 HCAPLUS Full-text
DOCUMENT NUMBER: 35:30348
ORIGINAL REFERENCE NO.: 35:4764c-g
TITLE: Synthesis of 6,8-dimethoxy-3-alkylisocoumarin. I. Alkylidenephthalide derivatives. (Synthesis of lobaritonide methyl ether)
AUTHOR(S): Nogami, Hisasi
SOURCE: Yakugaku Zasshi (1941), 61, 46-51(in German, 21-4)
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

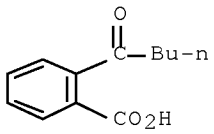
AB Treating 45 g. 3-ethylidenephthalide in 135 cc. benzene with NO2 in the cold gave 14 g. 3-nitroethylidenephthalide (I), C10H7O4N, m. 124°. Treating 2 g. I with 8 g. HI (d. 1.7) and 1 g. P gave 1 g. 3-methylisocoumarin (II), C10H8O2, m. 73-4°. 3-(α- Nitropropylidene)phthalide (prepared as above), HI and P when treated as indicated above gave 3-ethylisocoumarin, m. 76-7°. Heating of 20 g. 3,5-dimethoxyphthalic anhydride, 18 g. (BuCO)2O and 12 g. BuCO2Na on the oil bath at 185-210° for 2 hrs. gave 4 g. 4,6-dimethoxy-3- butylidenephthalide (III), C14H16O4, m. 126-7°, and the mother liquor gave 5,7-dimethoxy-3-butylidenephthalide, C14H16O4, m. 99°, and 3,5-dimethoxy-2-carboxyvalerophenone, C14H18O5, m. 134°. Hydrolysis of III in acetone with concentrated HCl, followed by the decarboxylation with Cu dust, gave 2,4-dimethoxyvalerophenone (IV), C13H18O3, m. 38.5°. Heating 10 g. resorcinol with 14 g. BuCO2H and 20 g. ZnCl2 gave 9 g. 2,4-dihydroxyvalerophenone, C11H14O3, m. 63°; semicarbazone, m. 175°. Methylation of the above compound with MeI gave IV. Heating 7.5 g. 3,5-dimethoxyphthalic anhydride, 4.7 g. anhydrous EtCO2H and 3.5 g. EtCO2Na on the oil bath at 170-80° for 1.5 hrs. gave 1.5 g. 5,7-dimethoxy-3-ethylidenephthalide, C12H12O4, m. 145°; 3,5-dimethoxy-2-carboxypropiophenone, C12H14O5, m. 158°. Decarboxylation of the above compound with Cu dust gave 3,5- dimethoxypropiophenone, m. 34-5°; semicarbazone, m. 130-1°. The other compds. obtained in the above reaction are 4,6-dimethoxy-3- ethylidenephthalide, C12H12O4, m. 185°, and 2,4-dimethoxy-6-carboxypropiophenone, C12H12O5, m. 160°. Decarboxylation of the above compound with Cu dust gave 2,4-dimethoxypropiophenone (V), m. 75°; semicarbazone, m. 205°. Methylation of 2,4-(HO)2C6H3COPr with MeI gave V.

IT 855469-97-5P, Benzoic acid, 2,4-dimethoxy-6-valeryl-
RL: PREP (Preparation)
(preparation of)

RN 855469-97-5 HCAPLUS
CN Benzoic acid, 2,4-dimethoxy-6-(1-oxopentyl)- (CA INDEX NAME)



L28 ANSWER 39 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1938:24255 HCAPLUS Full-text
DOCUMENT NUMBER: 32:24255
ORIGINAL REFERENCE NO.: 32:3361f-g
TITLE: Constituents of the fruits of Ligusticum acutilobum. III
AUTHOR(S): Kariyone, T.; Kotani, M.
SOURCE: Yakugaku Zasshi (1937), 57, 183-4
From: Chem. Zentr. 1937, II, 4051
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. C. A. 31, 2583.5. Of the compds. described in the earlier paper, ligusticumic acid and its lactone proved to be valerophenone-o-carboxylic acid and butylidenephthalide, resp. (cf. Noguchi and Kawanami, preceding abstract).
IT 550-37-8P, Benzoic acid, o-valeryl-
RL: PREP (Preparation)
(preparation of)
RN 550-37-8 HCAPLUS
CN Benzoic acid, 2-(1-oxopentyl)- (CA INDEX NAME)



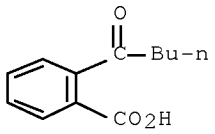
L28 ANSWER 40 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1938:24253 HCAPLUS Full-text
DOCUMENT NUMBER: 32:24253
ORIGINAL REFERENCE NO.: 32:3360d-h
TITLE: Chemical constituents of the Umbelliferae. IV. Constituents of Ligusticum acutilobum. 2
AUTHOR(S): Noguchi, Takami; Kawanami, Minoru
SOURCE: Yakugaku Zasshi (1937), 57, 196-208
From: Chem. Zentr. 1937, II, 4050-1
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Valerophenone-o-carboxylic acid (I), from butylidenephthalide (II) and alc. KOH (not pure because of lactonization), yellowish oil, b2 168-75°, gives with H2NCONHNH2.AcOH in alc. 1- butylphthalazonecarboxamide (III), m. 126°, which is converted by concentrated HCl on the water bath into 1-butylphthalazone, m.

155°, also formed from I and N2H4.H2O. Butylphthalamidine, from III with Zn and HCl, m. 85-6°. Me ester of I, from I and H2SO4 in MeOH, yellowish, b1.5 133-4°, d420 1.0803, nD20 1.51171. o-(Hydroxyamyl)benzoic acid, from I with H and PtO2 in AcOH. Amide of I, from II healed with alc. NH3, m. 134°. 1-Propylphthalazone, m. 163-4°, is obtained from N2H4.H2O and butyrophenone-o-carboxylic acid (from propylidenephthalide and alc. KOH), m. 88-9°. The ligusticumic acid obtained by Kariyone and Kotani (see below) from the ethereal oil of the fruits of L. acutilobum is I and ligusticumolactone is II. The crude acid also contains sedanonic acid (IV), for reduction with H and PtO2 in AcOH gives butylphthalide and dihydrosedanonic acid (semicarbazone, m. 180°). Me ester of IV, b2.5 132-3°, d420 1.0326, nD20 1.48088. 1-Butyl-Δ5,10-tetrahydrophthalazone, from IV and N2H4.H2O, m. 136°. The acid is not present as esters of dodecanol and tetradecanol, which probably are in the form of acetates, for AcOH is found in the saponification liquid. As the com. drug from the root of L. acutilobum is generally sprayed with camphor oil during storage, the greenish brown oil obtained from the roots by extraction with ether was again investigated; it contained in the acid portion palmitic, stearic, arachidic, linolic and oleic acids, in the other portion safrole, bergaptene, dodecanol, tetradecanol, butylphthalide, I, AcOH and esters of palmitic and linolic acid but no camphor.

IT 550-37-8, Benzoic acid, o-valeryl-
(and derivs.)

RN 550-37-8 HCAPLUS

CN Benzoic acid, 2-(1-oxopentyl)- (CA INDEX NAME)



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FILE 'REGISTRY' ENTERED AT 15:42:47 ON 15 AUG 2008

L1 STR
L2 11 S L1
L3 STR L1
L4 12 S L3
L5 233 S L3 FUL
L6 STR L3
L7 105 SEARCH L6 SUB=L5 FUL
L8 STR L6
L9 17 SEARCH L8 SUB=L5 FUL

FILE 'HCAPLUS' ENTERED AT 15:51:29 ON 15 AUG 2008

L10 2 S L9

FILE 'HCAPLUS' ENTERED AT 15:52:18 ON 15 AUG 2008

FILE 'REGISTRY' ENTERED AT 15:53:14 ON 15 AUG 2008

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L11          88 S L7 NOT L9

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L12          25 S L11
L13          24 S L12 NOT L10
                E SALMON R/AU
                E SALMON ROGER/AU
L14         219 S E3 OR SALMON ROGER ?/AU OR SALMON R/AU OR SALMON R ?/AU
                E CROWLEY P/AU
L15         150 S E3 OR E8 OR E10 OR E12 OR E14-E16
L16          19 S L14 AND L15

     FILE 'REGISTRY' ENTERED AT 15:58:54 ON 15 AUG 2008
L17         128 S L5 NOT (L7 OR L9)

     FILE 'HCAPLUS' ENTERED AT 15:59:07 ON 15 AUG 2008
L18          28 S L17
L19           3 S (L14 OR L15) AND L18
L20          17 S (L16 OR L19) NOT (L10 OR L13)

     FILE 'REGISTRY' ENTERED AT 16:17:56 ON 15 AUG 2008
L21             STR
L22           2 S L21
L23             STR L21
L24           6 S L23
L25         128 S L23 FUL
                SAVE TEMP L25 RICC826FUL/A
L26             STR L21
L27          38 SEARCH L26  SUB=L25 FUL

     FILE 'HCAPLUS' ENTERED AT 16:19:57 ON 15 AUG 2008
L28          40 S L27

     FILE 'HCAPLUS' ENTERED AT 16:20:31 ON 15 AUG 2008

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DICTIONARY FILE UPDATES:  14 AUG 2008  HIGHEST RN 1041071-62-8

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L29 90 L25 NOT L27

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FILE COVERS 1907 - 15 Aug 2008 VOL 149 ISS 8
FILE LAST UPDATED: 14 Aug 2008 (20080814/ED)

HCAplus now includes complete International Patent Classification (IPC)
reclassification data for the second quarter of 2008.

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This file contains CAS Registry Numbers for easy and accurate
substance identification.

L30 48 L29

=> s l30 not l28
L31 43 L30 NOT L28

=> d scan

L31 43 ANSWERS HCAPLUS COPYRIGHT 2008 ACS on STN
CC 35-6 (Synthetic High Polymers)
Section cross-reference(s): 22
TI Esterolytic activity of poly(1-methyl-4- and -5-vinylimidazole) in water
ST polyvinylimidazole esterolysis catalyst; carboxyphenyl alkanoate
esterolysis kinetics; enzyme analog esterolysis kinetics
IT Kinetics of hydrolysis
(of esters, in presence of poly(methylvinylimidazole))
IT Hydrolysis catalysts
(poly(methylvinylimidazole), for esters)
IT 56662-93-2 56662-95-4
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for hydrolysis of carboxyphenylalkanoate)
IT 2345-34-8 16358-93-3 56670-30-5 56670-31-6 56670-32-7
56670-33-8
RL: RCT (Reactant); RACT (Reactant or reagent)

(hydrolysis of, in presence of poly(methylvinylimidazole), kinetics of)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

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27433844 PD=<OCTOBER 12, 2006
(PD=<20061012)
L32 41 L31 AND PD=<OCTOBER 12, 2006

=> d scan

L32 41 ANSWERS HCAPLUS COPYRIGHT 2008 ACS on STN
CC 10-1 (Microbial Biochemistry)
Section cross-reference(s): 25
TI Structures and antimicrobial activity of peniophorin A and B, two polyacetylenic antibiotics from Peniophora affinis Burt
ST antibiotic peniophorin Peniophora
IT Peniophora affinis
(antibiotics peniophorins A and B from)
IT Molecular structure, natural product
(of peniophorin A)
IT Nomenclature, new natural products
(peniophorin A)
IT Nomenclature, new natural products
(peniophorin B)
IT Fungicides and Fungistats
(peniophorins A and B)
IT Antibiotics
(polyacetylenic, from Peniophora affinis, peniophorins A and B)
IT 75217-61-7 75217-62-8
RL: BIOL (Biological study)
(antibiotic, from Peniophora affinis)
IT 75235-25-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):.

L32 41 ANSWERS HCAPLUS COPYRIGHT 2008 ACS on STN
CC 10 (Organic Chemistry)
TI Fulvic acid: its structure and relationship to citromycetin and fusarubin
IT Fulvic acid
(structure of, and its relation to citromycetin and fusarubin)
IT 479-66-3
(Derived from data in the 6th Collective Formula Index (1957-1961))
IT 504-31-4, 2H-Pyran-2-one
(derivs.)
IT 109656-02-2, 1H-Naphtho[2,3-c]pyran-5,10-dione, 3,4-dihydro-3,6,9-trihydroxymethoxy-3-methyl-
(fusarubin and)
IT 4394-72-3P, 2,4,6-Octatrienoic acid, 5-hydroxy-3,7-dimethyl-, δ-lactone 95730-85-1P, 1H,10H-Pyrano[4,3-b][1]benzopyran-9-carboxylic acid, 7,8-dihydroxy-3-methyl-10-oxo- 95730-85-1P, 1H,10H-Pyrano[4,3-b][1]benzopyran-9-carboxylic acid, 7,8-dihydroxy-3-methyl-10-oxo-, anhydrofulvic acid 109100-85-8P, Benzoic acid, 2,3,5-trihydroxy-6-[2-(hydroxymethyl)-3,5-dioxohexanoyl]-
RL: PREP (Preparation)
(preparation of)

IT 478-60-4, Citromycetin 1702-77-8, Fusarubin
(structure of)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):.

L32 41 ANSWERS HCAPLUS COPYRIGHT 2008 ACS on STN
CC 1-3 (Pharmacology)
Section cross-reference(s): 7
TI Receptor mapping by comparative molecular field analysis of phospholipase A2 inhibitors
ST phospholipase A2 inhibitor structure based design
IT Inflammation inhibitors
(design; receptor mapping by comparative mol. field anal. of phospholipase A2 inhibitors in relation to drug design)
IT Molecular structure-biological activity relationship
(receptor mapping by comparative mol. field anal. of phospholipase A2 inhibitors in relation to drug design)
IT 9001-84-7, Phospholipase A2
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(receptor mapping by comparative mol. field anal. of phospholipase A2 inhibitors in relation to drug design)
IT 167775-07-7 167775-08-8 167775-09-9 167775-10-2
167775-11-3 167775-12-4 167775-13-5 167775-14-6 167775-15-7
167775-16-8 167775-17-9 167775-18-0 167775-19-1 167775-20-4
167775-21-5 167775-22-6 167775-23-7 167775-24-8 167775-25-9
167775-26-0 167775-27-1 167775-28-2
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(receptor mapping by comparative mol. field anal. of phospholipase A2 inhibitors in relation to drug design)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):.

L32 41 ANSWERS HCAPLUS COPYRIGHT 2008 ACS on STN
CC 35 (Noncondensed Aromatic Compounds)
TI Polyacetylene compounds. CIX. Synthesis of naturally occurring, aromatic substituted acetylene compounds
IT Antispasmodics
(phenoxyalkyl amines as)
IT 1,3-Isochromandione, 3-(2-butynyl)-
2-Hexene-4,6-diyn-1-ol, 7-(m-hydroxyphenyl)-, diacetate
RL: PREP (Preparation)
IT 7387-96-4 10429-31-9 10429-32-0 13072-40-7 95159-95-8
(Derived from data in the 7th Collective Formula Index (1962-1966))
IT 84-72-0P, Phthalic acid, ethyl ester, ester with Et glycolate 84-72-0P, Glycolic acid, ethyl ester, ester with Et phthalate 3570-28-3P, Isocoumarin, 3-(2-butynyl)- 4368-08-5P, o-Anisic acid, 6-(2,4-hexadiynyl)-, methyl ester 7347-83-3P, Benzophenone, 2-[2-(dimethylamino)propoxy]-, hydrochloride 7347-84-4P, Benzophenone, 2-[2-(diethylamino)propoxy]-, hydrochloride 7347-85-5P, Ammonium, [2-(o-benzoylphenoxy)-1-methylethyl]diethylmethyl, iodide 7347-86-6P, Piperidinium, 1-[2-(2-benzoylphenoxy)-1-methylethyl]-1-methyl-, iodide 7347-87-7P, Ammonium, diethylmethyl[1-methyl-2-[(α-phenyl-o-tolyl)oxy]ethyl], iodide 7347-88-8P, Ammonium, tert-butyldimethyl[1-methyl-2-[(α-phenyl-o-tolyl)oxy]ethyl], iodide 7347-89-9P, Pyrrolidinium, 1-methyl-1-[1-methyl-2-[2-(phenylmethyl)phenoxy]ethyl]-,

iodide 7347-90-2P, Piperidinium, 1-ethyl-1-[1-methyl-2-[2-(phenylmethyl)phenoxy]ethyl]-, iodide 7347-91-3P, Triethylamine, 1-methyl-2-[(α-phenyl-o-tolyl)oxy]-, hydrochloride 7347-92-4P, Ammonium, trimethyl[1-methyl-2-[(α-phenyl-o-tolyl)oxy]ethyl], p-toluenesulfonate 7350-01-8P, Piperidinium, 1-methyl-1-[1-methyl-2-[2-(phenylmethyl)phenoxy]ethyl]-, salt with 4-methylbenzenesulfonic acid (1:1) 7387-95-3P, Ammonium, [3-[(α-hydroxy-α,α-diphenyl-o-tolyl)oxy]propyl]trimethyl, p-toluenesulfonate 7387-97-5P, Piperidinium, 1-[1-methyl-2-[2-(phenylmethyl)phenoxy]ethyl]-1-propyl-, sulfate (1:1) 10398-89-7P, 3-Isochromancarboxylic acid, 3-(2-butynyl)-1,4-dioxo-, ethyl ester 10398-89-7P, Benzoic acid, o-(2-carboxy-2-hydroxy-4-hexynoyl)-, δ-lactonet, Et ester 10401-06-6P, Anisole, 2-bromo-3-(2,4-hexadiynyl)- 10401-07-7P, 2,4-Hexadiynophenone, 2'-bromo-3'-methoxy- 10401-08-8P, 1,3-Dioxolane, 2-(2-bromo-3-methoxyphenyl)-2-(1,3-pentadiynyl)- 10401-09-9P, Cinnamic acid, m-hydroxy-, ethyl ester, benzoate 10401-10-2P, Propiolic acid, (m-hydroxyphenyl)- 10401-11-3P, Phenol, m-ethynyl- 10401-14-6P, Benzoic acid, o-(carboxyglycoloyl)-, δ-lactonet, Et ester 10401-14-6P, 3-Isochromancarboxylic acid, 1,4-dioxo-, ethyl ester 10401-15-7P, Benzoic acid, o-(2-hydroxy-4-hexynoyl)-, δ-lactone 10401-16-8P, 2,4-Hexadiyn-1-ol, 1-(2-bromo-3-methoxyphenyl)- 10401-17-9P, m-Anisaldehyde, 2-bromo-, (2,4-dinitrophenyl)hydrazone 10401-18-0P, m-Anisaldehyde, 2-bromo- 10401-19-1P, Anisole, 2-bromo-3-(dichloromethyl)- 10401-21-5P, o-Anisic acid, 6-(2,4-hexadiynoyl)-, methyl ester 10401-25-9P, Benzophenone, 2-[2-(dipropylamino)propoxy]-, hydriodide 10401-26-0P, Benzophenone, 2-[2-(dibutylamino)propoxy]-, hydriodide 10429-12-6P, Benzhydrol, 2-(3-piperidinopropoxy)-, hydrobromide 10429-13-7P, Methanol, [o-[3-(dimethylamino)propoxy]phenyl]diphenyl-, hydrochloride 10429-14-8P, Methanol, [o-[3-(diethylamino)propoxy]phenyl]diphenyl-, hydrobromide 10429-15-9P, Ammonium, dibutyl[3-[(α-hydroxy-α-phenyl-o-tolyl)oxy]-propyl]methyl, iodide 10429-16-0P, Piperidinium, 1-[3-[(α-hydroxy-α-phenyl-o-tolyl)oxy]propyl]-1-methyl-, iodide 10429-25-1P, Benzophenone, 2-[3-(dimethylamino)propoxy]-, hydrobromide 10429-26-2P, Benzophenone, 2-[3-(diethylamino)propoxy]-, phosphate 10429-27-3P, Benzophenone, 2-[3-(dipropylamino)propoxy]-, hydriodide 10429-28-4P, Benzophenone, 2-[3-(dibutylamino)propoxy]-, hydrobromide 10429-30-8P, Benzaldehyde, o-[3-(dimethylamino)propoxy]- 10429-33-1P, Benzhydrol, 2-[3-(dipropylamino)propoxy]-, hydrochloride 10429-34-2P, Benzhydrol, 2-[3-(dibutylamino)propoxy]-, hydrobromide 10429-35-3P, Propylamine, 2-[(α-phenyl-o-tolyl)oxy]-, hydrochloride 10429-37-5P, Dipropylamine, N-[1-methyl-2-[(α-phenyl-o-tolyl)oxy]ethyl]-, hydrochloride 10429-38-6P, Dibutylamine, N-[1-methyl-2-[(α-phenyl-o-tolyl)oxy]ethyl]-, hydrobromide 10429-39-7P, Diethylamine, N,1,1,1'-tetramethyl-2'-[(α-phenyl-o-tolyl)oxy]-, hydrobromide 10429-40-0P, Pyrrolidine, 1-[1-methyl-2-[(α-phenyl-o-tolyl)oxy]ethyl]-, phosphate 10429-41-1P, Piperazine, 1-methyl-4-[1-methyl-2-[(α-phenyl-o-tolyl)oxy]ethyl]-, dihydrochloride 10429-42-2P, Piperidine, 1-[2-[(α-phenyl-o-tolyl)oxy]propyl]-, hydrochloride 10429-44-4P, Ethylamine, 2-[(α-phenyl-o-tolyl)oxy]- 10429-51-3P, Propylamine, N,N-diethyl-3-[(α-phenyl-o-tolyl)oxy]-, hydrochloride 10429-52-4P, Propylamine, 3-[[α-(p-chlorophenyl)-o-tolyl]oxy]-N,N-diethyl-, hydriodide 10429-55-7P, Piperazinium, 1,1-dimethyl-4-[1-methyl-2-[(α-phenyl-o-tolyl)oxy]ethyl]-, iodide 10429-56-8P, Dibutylamine,

N-[3-[[α-(p-chlorophenyl)-o-tolyl]oxy]propyl]-, hydrochloride 10429-57-9P, Phenethylamine, α-methyl-N-[2-[(α-phenyl-o-tolyl)oxy]ethyl]-, hydrochloride 10429-58-0P, 2-Indanamine, N-[2-[(α-phenyl-o-tolyl)oxy]ethyl]-, hydrochloride 10429-59-1P, Acetamide, N-2-indanyl-2-[(α-phenyl-o-tolyl)oxy]- 10429-60-4P, Acetamide, 2-(p-hydroxyphenyl)-N-[2-[(α-phenyl-o-tolyl)oxy]ethyl]- 10429-61-5P, Phenol, p-[2-[[2-[(α-phenyl-o-tolyl)oxy]ethyl]amino]ethyl]-, hydrochloride 10429-62-6P, p-Toluenesulfonamide, N-(2-hydroxyethyl)-N-(α-methylphenethyl)-, p-toluenesulfonate 10429-63-7P, p-Toluenesulfonamide, N-[2-(o-benzoylphenoxy)ethyl]-N-(α-methylphenethyl)- 10429-64-8P, Benzophenone, 2-[2-[(α-methylphenethyl)amino]ethoxy]-, hydrochloride 10446-32-9P, 2-Propanone, [p-(p-hydroxyphenoxy)phenyl]- 10571-21-8P, Benzophenone, 2-(2-piperidinopropoxy)-, hydrobromide 10602-06-9P, Benzoic acid, m-ethynyl-, methyl ester 13002-43-2P, Ammonium, [3-[(α-hydroxy-α-phenyl-o-tolyl)oxy]propyl]trimethyl, p-toluenesulfonate 13002-44-3P, Ammonium, diethyl[3-[(α-hydroxy-α-phenyl-o-tolyl)oxy]propyl]methyl, p-toluenesulfonate 13002-45-4P, Ammonium, [3-[(α-hydroxy-α-phenyl-o-tolyl)oxy]propyl]methyldipropyl, p-toluenesulfonate 13061-65-9P, m-Anisaldehyde, 2-bromo-, oxime 13072-41-8P, Morpholine, 4,4'-(2-bromo-3-methoxybenzylidene)di- 13259-72-8P, Piperidine, 1-[1-methyl-2-[(α-phenyl-o-tolyl)oxy]ethyl]-, hydrochloride 13259-73-9P, Butylamine, N,N-dimethyl-4-[(α-phenyl-o-tolyl)oxy]-, hydrochloride 13381-25-4P, Benzophenone, 2-(3-piperidinopropoxy)-, hydrobromide 93948-74-4P, Benzhydrol, 2-[3-(dimethylamino)propoxy]-, phosphate (salt) 94299-21-5P, 1,2-Pentanedione, 1-[p-(p-methoxyphenoxy)phenyl]-, 2-oxime 94876-38-7P, Benzhydrol, 2-[3-(diethylamino)propoxy]-, phosphate (salt) 879653-64-2P, Ammonium, diethyl[3-(α-hydroxy-α,α-diphenyl-o-tolyl)propyl]methyl, p-toluenesulfonate
RL: PREP (Preparation)
(preparation of)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):.

L32 41 ANSWERS HCAPLUS COPYRIGHT 2008 ACS on STN
CC 30-20 (Terpenes and Terpenoids)
TI Efficient Construction of the Oxatricyclo[6.3.1.00,0]dodecane Core of Komaroviquinone Using a Cyclization/Cycloaddition Cascade of a Rhodium Carbenoid Intermediate
ST oxatricyclododecane core komaroviquinone prepn cyclization cycloaddn cascade rhodium carbenoid
IT Cyclization
Cyclization catalysts
Cycloaddition reaction
(efficient construction of oxatricyclo[6.3.1.00,0]dodecane core of komaroviquinone using a cyclization/cycloaddn. cascade of a rhodium carbenoid intermediate)
IT 15956-28-2, Dirhodium tetraacetate
RL: CAT (Catalyst use); USES (Uses)
(efficient construction of oxatricyclo[6.3.1.00,0]dodecane core of komaroviquinone using a cyclization/cycloaddn. cascade of a rhodium carbenoid intermediate)
IT 485835-92-5P, Komaroviquinone
RL: PNU (Preparation, unclassified); PREP (Preparation)

(efficient construction of oxatricyclo[6.3.1.00,0]dodecane core of komaroviquinone using a cyclization/cycloaddn. cascade of a rhodium carbenoid intermediate)

IT 764-59-0, 5-Hexenal 2065-66-9, Methyl triphenylphosphonium iodide 4376-18-5, Phthalic acid monomethyl ester 86549-27-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(efficient construction of oxatricyclo[6.3.1.00,0]dodecane core of komaroviquinone using a cyclization/cycloaddn. cascade of a rhodium carbenoid intermediate)

IT 18435-67-1P 53589-52-9P 288296-26-4P 864718-96-7P 864718-97-8P 864718-98-9P 864718-99-0P 864719-00-6P 864719-01-7P 864719-04-0P 864719-05-1P 864719-06-2P 864719-07-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(efficient construction of oxatricyclo[6.3.1.00,0]dodecane core of komaroviquinone using a cyclization/cycloaddn. cascade of a rhodium carbenoid intermediate)

IT 864719-02-8P 864719-03-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(efficient construction of oxatricyclo[6.3.1.00,0]dodecane core of komaroviquinone using a cyclization/cycloaddn. cascade of a rhodium carbenoid intermediate)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):.

L32 41 ANSWERS HCAPLUS COPYRIGHT 2008 ACS on STN
CC 35-6 (Synthetic High Polymers)
Section cross-reference(s): 22
TI Esterolytic activity of poly(1-methyl-4- and -5-vinylimidazole) in water
ST polyvinylimidazole esterolysis catalyst; carboxyphenyl alkanoate esterolysis kinetics; enzyme analog esterolysis kinetics
IT Kinetics of hydrolysis
(of esters, in presence of poly(methylvinylimidazole))
IT Hydrolysis catalysts
(poly(methylvinylimidazole), for esters)
IT 56662-93-2 56662-95-4
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for hydrolysis of carboxyphenylalkanoate)
IT 2345-34-8 16358-93-3 56670-30-5 56670-31-6 56670-32-7 56670-33-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrolysis of, in presence of poly(methylvinylimidazole), kinetics of)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> => d stat que l46
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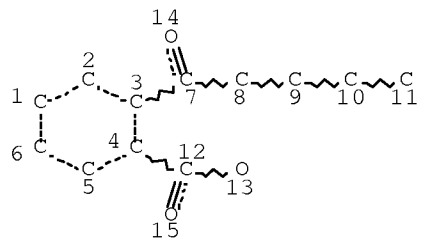

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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE
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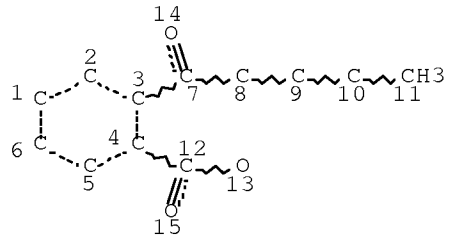

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE
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L36 1893 SEA FILE=HCAPLUS ABB=ON PLU=ON ZHAO X/AU OR ZHAO X ?/AU OR ZHAO XING/AU OR ZHAO XING KAI/AU OR ZHAO XINGKAI/AU
L37 172 SEA FILE=HCAPLUS ABB=ON PLU=ON "MA XISHENG"/AU OR MA XI/AU OR MA XI ?/AU
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L43 2 SEA FILE=HCAPLUS ABB=ON PLU=ON L38 AND L40
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L45 4 SEA FILE=HCAPLUS ABB=ON PLU=ON L44 AND PATENT/DT
L46 3 SEA FILE=HCAPLUS ABB=ON PLU=ON (L39 OR L41 OR L42 OR L43 OR

L45) NOT (L28 OR L27)

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L46 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:549504 HCAPLUS Full-text
TITLE: Pharmaceutical composition having anti-inflammatory and analgesic effects
INVENTOR(S): Hu, Yingqing; Yang, Wenbin; Zhao, Xingkai; Qin, Hua
PATENT ASSIGNEE(S): Beijing Team Academy of Pharmaceutical Science, Peop. Rep. China
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu
CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1682913	A	20051019	CN 2005-10051390	20050309 <--

PRIORITY APPLN. INFO.: CN 2005-10051390 20050309
AB The title composition comprises Daemonorops draco and borneol at a weight ratio of (1-9):1, preferably (4-9):1. It has anti-inflammatory and analgesic effects and can be prepared into the forms of oral preparations such as tablet, capsule, granule, dripping pill, powder, and pill; as well as topical preparation such as plaster.

L46 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:1350280 HCAPLUS Full-text
DOCUMENT NUMBER: 144:88042
TITLE: Preparation of (S)-2-(1-hydroxypentyl)benzoic acid salts for treatment of cardiac ischemia, cerebral ischemia, and thrombotic diseases
INVENTOR(S): Liu, Quanzhi; Yang, Wenbin; Qin, Hua; Zhao, Xingkai
PATENT ASSIGNEE(S): Team Academy of Pharmaceutical Science, Peop. Rep. China
SOURCE: PCT Int. Appl., 34 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005123651	A1	20051229	WO 2005-CN102	20050124 <--

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
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RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CN 1594270 A 20050316 CN 2004-10048268 20040617 <--

PRIORITY APPLN. INFO.: CN 2004-10048268 A 20040617

OTHER SOURCE(S): MARPAT 144:88042

AB The title (S)-2-(1-hydroxypentyl)benzoic acid salts were prepared for treatment of cardiac ischemia, cerebral ischemia, and thrombotic diseases, and improving the circulation in heart and brain. For example, the Li, Na, K, Zn, Mg, tert-butylamine, benzylamine, and 1,2- dibenzylethylenediamine salts were prepared from (S)-2-(1- hydroxypentyl)benzoic acid and the corresponding base. The results showed that the compds. are useful as anticoagulants. Formulations containing the title compound as an active ingredient were also described.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L46 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:216786 HCAPLUS Full-text

DOCUMENT NUMBER: 142:285151

TITLE: N, N'-dibenzyl ethylenediamine salt of 2-(alpha-hydroxypentyl) benzoic acid and its preparing process and usage

INVENTOR(S): Yang, Wenbin; Qin, Hua; Zhao, Xingkai; Ma, Xisheng

PATENT ASSIGNEE(S): Team Academy of Pharmaceutical Science, Peop. Rep. China

SOURCE: PCT Int. Appl., 24 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Chinese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005021481	A1	20050310	WO 2004-CN102	20040209 <--

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CN 1523003 A 20040825 CN 2003-156495 20030901 <--

PRIORITY APPLN. INFO.: CN 2003-156495 A 20030901

AB N,N'-dibenzyl ethylenediamine salt of 2-(alpha-hydroxypentyl) benzoic acid, which has significant effects in inhibiting blood platelet aggregation and improving cerebral circulation as anti-ischemic agents in the treatment of brain and heart ischemia, and cardiac or cerebral arterial embolism with good appearance, phys. state and wet stability, is provided. The preparing process of the salt, the pharmaceutical composition containing it as active component and its use in preparing medicine against brain and heart ischemia, cardiac or cerebral arterial embolism and the like are also disclosed.

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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=> d his ful l21-


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L46           3 SEA ABB=ON  PLU=ON  (L39 OR L41 OR L42 OR L43 OR L45) NOT (L28
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     FILE HOME

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     Property values tagged with IC are from the ZIC/VINITI data file
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     STRUCTURE FILE UPDATES:   14 AUG 2008  HIGHEST RN 1041071-62-8
     DICTIONARY FILE UPDATES:  14 AUG 2008  HIGHEST RN 1041071-62-8

     New CAS Information Use Policies, enter HELP USAGETERMS for details.

     TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

       Please note that search-term pricing does apply when
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http://www.cas.org/support/stngen/stndoc/properties.html

FILE HCAPLUS

FILE COVERS 1907 - 15 Aug 2008 VOL 149 ISS 8
FILE LAST UPDATED: 14 Aug 2008 (20080814/ED)

HCAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

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This file contains CAS Registry Numbers for easy and accurate substance identification.

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